



INVITED PRESENTERS YOUNG INVESTIGATOR FORUM: GROWN The BIO-FUTURE
THE ONLINE VIRTUAL SESSION PROJECT on Tue, 1 June, 2021

“SMART NANO-MATERIALS/SYSTEMS MULTIFUNCTIONALITY STRATEGY FROM NATURE”

THE E-MRS INVITED ORGANIZERS/CHAIRS

PhD student Toshifumi Imajo, University of Tsukuba, Japan

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Toshifumi Imajo is a PhD student of University of Tsukuba supervised by Assoc. Prof. Dr. Kaoru Toko. His research interests are low-temperature synthesis of polycrystalline Ge thin films on insulators and its applications to thin-film transistors and solar cells. In particular, he developed advanced solid-phase crystallization (SPC) technique, which enables us to form the high-quality polycrystalline Ge thin film on glass and plastic substrates. Using this technique, he has continuously updated the highest carrier mobility among the semiconductor thin films directly formed on insulators at low temperatures. He has 10 papers, 6 of which are the first authors. Recently, his oral presentation was selected for Highlight lecture in the JSAP Meeting, the most prominent conference for applied physics in Japan.



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Ana Arché Núñez is a PhD student at the Complutense University of Madrid, supervised by the Assistant Researcher Dr. Teresa González Pérez and the Tenured Scientist Dr. María Concepción Serrano López-Terradas. Her research interests are the synthesis and characterization of nanomaterials and their *in vitro* biological response. Under the framework of the ByAxon project, she fabricates low-disturbance flexible nanostructured planar electrodes based on vertical metallic nanowires standing over a flexible Au base, as well as sharp nanostructured metallic electrodes within the context of BiSURE project. With those electrodes, she expects to perform extracellular

and intracellular measurements, respectively. Some important electrodes' fabrication techniques that she is familiar with are the anodization of aluminum to generate nanoporous templates and template-assisted electrodeposition technique to obtain nanowires. She is also acquainted with cell cultures and the post treatment and analysis of the cells to study the cells viability, differentiation and morphology. She has received an I+D+i (RETOS) fellowship under the project DPI2017-90058-R and has been awarded with the Materplat 2018 Award for her Master thesis work. Finally, she is a coauthor of two published articles and three more in preparation.

***THE E-MRS INVITED SCIENTIFIC ADVISORS TO HELD
YOUNG INVESTIGATOR FORUM***

***Dr. María Concepción Serrano López-Terradas, ICMM-CSIC, Madrid, Spain
Dr. María Teresa González Pérez, IMDEA Nanoscience, Madrid, Spain***



María Concepción Serrano López-Terradas

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María Concepción Serrano López-Terradas is a Tenured Scientist at the Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) working in the research topic of Materials for Health in Spain. Her research focuses on the design and development of biomaterials for biomedical applications including a wide range of materials (ceramics, polymers, hydrogels, elastomers, carbon nanotubes, graphene, etc) and applications (neural regeneration, congenital cardiovascular pathologies, atherosclerosis, osteoporosis, bone cancer). She has been responsible for the set-up and functioning of the first cell and tissue culture laboratories at the ICMM-CSIC (one of biosafety level 2). She has been granted with a FPU predoctoral fellow from the MEC of Spain (2003-2006), a postdoctoral contract abroad from the MICINN of Spain (2008-2010), a Juan de la Cierva postdoctoral contract from the MINECO of Spain (2010-2013) and a Miguel Servet I postdoctoral contract from the ISCIII of Spain (2014-2017). She has been principal investigator of the project MAT2016-78857R from MINECO (2017-2020, 121 k€) and CP13/0060 from ISCIII of Spain (2014-2017, 120 k€), and work package leader of the WP3 in the European Project H2020 FET-OPEN-RIA ByAxon (210 k€). She has also been responsible for the creation of the Joint Research Unit of I+D+I with CSIC "Design and development of biomaterials for neural regeneration" of the Hospital Nacional de Paraplégicos in Toledo. Since March 1st, 2019, she is an Associate Editor of the journal "Bioactive Materials". She has co-authored over 60 publications in scientific journals of Q1, receiving more than 2,500 citations and a resulting h index of 30, and more than 70 communications to national and international conferences, besides being actively involved in outreach activities. Finally, she has got favorable recognition of 2 Sexenios de Investigación (2004-2015) by Comisión Nacional Evaluadora de la Actividad Investigadora (Ministerio de Ciencia, Innovación y Universidades) (06/06/2018) and 3 Quinquenios (Componente por Méritos Investigadores del Complemento Específico) (2003-2017) by CSIC (MINECO) (12/06/2018). Researcher [ID D-7442-2014](#), Scopus [ID 9244466100](#) and [ORCID 0000-0002-5010-644X](#).



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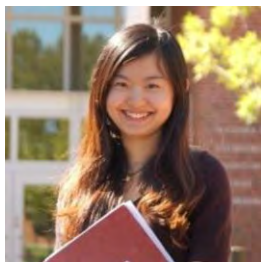
M. Teresa González got her PhD in Physics (2003) at the Universidad de Santiago de Compostela in Spain, awarded as Outstanding Doctorate. She is an expert in electrical transport properties of matter. She has worked in different

fields including superconductivity, molecular electronics, and more recently, the recording and stimulation of electric impulses at the nervous tissue. She worked as a postdoctoral researcher at the Universität Basel in Christian Schönenberger's group (2004-2008), and then joined the Fundación IMDEA Nanociencia in Madrid in 2008, where she continues to work. She is presently head of the IMDEA Neural Interfaces Laboratory. She has co-authored 46 scientific works with more than 1600 citations and an H-index of 21. She has participated in 5 European projects, and has been co-coordinator of the FET-OPEN ByAxon project (737116, 2017-2020). She has presented several invited talks, oral communications in more than 20 international conferences and workshops and posters in more than 30. Researcher ID [H-5527-2012](#), Scopus ID [57194289691](#), ORCID [0000-0002-7253-797X](#).

INVITED PRESENTERS YOUNG INVESTIGATOR FORUM

1. INVITED PRESENTATION Xiaohui Ju

10:20 (O.YIF.1)



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Research Area: bio-application of cerium oxide nanoparticles as future nanomedicine

Polymer coated cerium oxide nanoparticles as nanomedicine: synthesis, stability, activity, and cellular uptake

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Cerium oxide nanoparticles (CeNPs) possess multiple enzyme mimetic activities to scavenge reactive oxygen species (ROS) in the biological environment as potential nanomedicine. One of the biggest challenges for the biomedical applications of CeNPs is to maintain their colloidal stability and catalytic activity as enzyme mimetics after nanoparticles enter the human cellular environment. This work summarized our latest findings of the influences of CeNP surface properties on their colloidal stability, enzymatic activity, and cellular uptake. Near-spherical CeNPs stabilized via different hydrophilic polymers were prepared through a wet-chemical precipitation method. The mechanism of polymer-cerium oxide was studied in detail using model thin film systems and surface science techniques. The CeNPs interaction with the cell culture media was tested to confirm their colloidal stabilities. Cellular uptake of these CeNPs was characterized by a collective of spectroscopic and microscopic methods.

Our study showed that polymers attach to the surface of cerium oxide through a mutual charge transfer adsorption. By controlling the synthesis conditions, we can tune the surface oxidation states of synthesized CeNPs with the same core sizes, morphology, crystal structure, dispersity, and colloidal stability, with the only changing parameter being CeNPs surface oxidation state (Ce³⁺ percentage). We further investigated the performance of the synthesized CeNPs as enzyme mimetics, such as superoxide dismutase, catalase, peroxidase, and oxidase. It is shown that their enzyme mimetic behavior as well as their abilities are directly linked to their surface oxidation state. We found a strong correlation between CeNPs intrinsic surface properties and the extrinsic influences of the biological environment, such as the presence of biomacromolecules (protein corona formation) and solution properties (pH and ionic strength). We further examined their performance as antioxidants in vitro. Results showed no toxicity of these CeNPs for three different cell lines (osteoblasts, macrophages, and monocytes). A positive relation between the CeNPs surface oxidation state and their ability to reduce the intercellular ROS level is observed. Further microscopic and spectroscopic tests showed the location of these CeNPs during cellular uptake. These results showed that CeNPs could further be tuned by polymer coating to achieve its potential application as nanomedicine.



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Ana Arché Núñez is a PhD student at the Complutense University of Madrid, supervised by the Assistant Researcher Dr. Teresa González Pérez and the Tenured Scientist Dr. María Concepción Serrano López-Terradas. Her research interests are the synthesis and characterization of nanomaterials and their *in vitro* biological response. Under the framework of the ByAxon project, she fabricates low-disturbance flexible nanostructured planar electrodes based on vertical metallic nanowires standing over a flexible Au base, as well as sharp nanostructured metallic electrodes within the context of BiSURE project. With those electrodes, she expects to perform extracellular and intracellular measurements, respectively. Some important electrodes' fabrication techniques that she is familiar with are the anodization of aluminum to generate nanoporous templates and template-assisted electrodeposition technique to obtain nanowires. She is also acquainted with cell cultures and the post treatment and analysis of the cells to study the cells viability, differentiation and morphology. She has received an I+D+i (RETOS) fellowship under the project DPI2017-90058-R and has been awarded with the Materplat 2018 Award for her Master thesis work. Finally, she is a coauthor of two published articles and three more in preparation.

María Concepción Serrano López-Terradas is a Tenured Scientist at the Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) working in the research topic of Materials for Health in Spain. She has co-authored over 60 publications in scientific journals of Q1, receiving more than 2,500 citations and a resulting h index of 30.

María Teresa González Pérez is presently head of the IMDEA Nanoscience Neural Interfaces Laboratory. She has co-authored 46 scientific works with more than 1600 citations and an H-index of 21. She has participated in 5 European projects, and has been co-coordinator of the FET-OPEN ByAxon project (737116, 2017-2020).

Referred Journals Publication List

- (1) Calaresu, I, Hernandez, J, Rauti, R, Rodilla, B, Arché-Núñez, A, Perez, L, Camarero, J, Miranda, R, González, MT, Rodríguez, I, Scaini, D, Ballerini, L. Polystyrene Nanopillars with Inbuilt Carbon Nanotubes Enable Synaptic Modulation and Stimulation in Interfaced Neuronal Networks. *Advanced Materials Interfaces* 2002121 (2021).
- (2) Domínguez-Bajo, A, Rodilla, BL, Calaresu, I, Arché-Núñez, A, González-Mayorga, A, Scaini, D, Pérez, L, Camarero, J, Miranda, R, López-Dolado, E, González, MT, Ballerini, L, Serrano, MC. Interfacing Neurons with Nanostructured Electrodes Modulates Synaptic Circuit Features. *Advanced Biosystems* 4, 2000117, (2020).

Planar and sharp nanotechnology-based electrodes for neural activity recording and stimulation

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Neural activity can be measured or stimulated using electrodes that can be improved with nanotechnology advances. In this work, we propose the use of template-assisted electrodeposition technique to obtain, in a reproducible way, nanostructured metallic surfaces that can work as neural electrodes.

On one hand, planar electrodes are used in extracellular experiments and medical applications to register or stimulate neural activity. In the context of the ByAxon project, our results on the fabrication of low-disturbance flexible nanostructured planar electrodes based on vertical metallic nanowires standing over a flexible Au base will be presented. We have obtained low impedance electrodes by electrodeposition using anodic aluminium oxide templates fabricated at the laboratory, controlling the geometry of the electrode's nanostructured surface. Biocompatibility studies with these electrodes showed proper neural cell adhesion, growth and differentiation.

On the other hand, to perform intracellular in vitro recordings, patch-clamp technique is the most extended one. However, it damages the cell due to perforation size and medium exchange reducing life time when measuring. In this work, our progress in the fabrication of sharp nanostructured metallic electrodes based on the process described above, in order to improve the existing intracellular recordings, will be shown.

Work funded by H2020 R&D programme under grant agreement No. 737116 and I+D+I project DPI2017-90058-R



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Isabella Nymann Westensee is a PhD student at the Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Denmark, supervised by Brigitte Städler (Laboratory for Cell Mimicry). She is currently working in the research topic of cell mimicry, where the question of how structural and functional aspects of eukaryotic cells can be mimicked with bottom-up synthetic biology is of key interest, where hepatocytes serve as a key source of inspiration. The focus during the PhD until now has been on implementing energy generation in artificial cells, as well as establishing communication between artificial cells and hepatocytes by using both natural and synthetic subunits to incorporate function in hydrogel based cell-sized assemblies. Currently, she is co-author of four published articles and has two more in preparation.

Publication List

- (1) I. N. Westensee, E. Brodzkij, X. Qian, T. F. Marcelino, K. Lefkimiatis, B. Städler. Mitochondria Encapsulation in Hydrogel-based Artificial Cells as ATP Producing Subunits, *Small*, accepted.
- (2) X. Qian*, I. Westensee*, E. Brodzkij*, B. Städler, Cell mimicry as a bottom-up strategy for hierarchical engineering of nature-inspired entities. *WIREs Nanomed Nanobiotechnol.* 2020; e1683. (*Shared 1st author)
- (3) DE. Brodzkij, I. Westensee, M. Bertelsen, N. Gal, and B. Städler, Polymer – lipid hybrid vesicles and their interaction with HepG2 cells, *Small*, 2020, 16, 1906493.
- (4) Y. Zhang, N. Gal, F. Itel, I. N. Westensee, E. Brodzkij, D. Mayer, S. Stenger, M. Castellote-Borrell, T. Boesen, S. R. Tabaei, F. Höök, B. Städler, Hybrid vesicles as intracellular reactive oxygen species and nitric oxide generators, *Nanoscale*, 2019, 11, 11530–11541.

Communication between artificial cells and hepatocytes

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Aarhus University, Interdisciplinary Nanoscience Center (iNANO)

Artificial cells (ACs) aim to mimic certain structural and functional features of natural cells*, with the aim ranging from studying the origin of life to developing AC-based therapeutics to support cells and tissues with missing functions. There is a plethora of features to be mimicked of the mammalian cell in the construction of an AC, one of them being cell communication. Living cells communicate by secreting signaling molecules that can activate certain responses in neighboring cells. Multicellular organisms rely on this chemical signaling between individual cells to coordinate collective behaviors and responses to changes in the extracellular environment. Here, we are focusing on a one-way communication from ACs to HepG2 cells using small fluorescent compounds as messengers. The ACs were assembled using alginate hydrogel beads equipped with two different metalloporphyrins that mimic the catalytic function of certain CYP450 enzymes. One catalyzes the hydroxylation of coumarin to form 7-hydroxylation while the other one fulfills the dealkylation of resorufin ethyl ether to generate resorufin. The former was directly conjugated to the alginate polymer while the latter was encapsulated in liposomes before entrapping into the alginate beads. The biocatalytic activity of the ACs was optimized while ensuring that none of the compounds affected the viability of the HepG2 cells. Subsequently, the two products produced by the ACs (7-hydroxy coumarin and resorufin) could diffuse and be taken up by the receiving HepG2 cells, leading to an increase of cell mean fluorescence as a simple response. This effort showcases simultaneous communication between mammalian cells and two AC populations, facilitated through the use of metalloporphyrins as artificial enzymes. *Qian, X., Nymann Westensee, I., et al. Cell mimicry as a bottom-up strategy for hierarchical engineering of nature-inspired entities. *WIREs Nanomed Nanobiotechnol.* 2020;e1683.



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Anita Ioana Visan is a Postdoctoral researcher at National Institute for Lasers, Plasma and Radiation Physics (INFLPR), "Laser-Surface-Plasma Interactions" Laboratory, Lasers Department, Romania. Her career highlights involves: Materials science; surface engineering by UV excimer lasers and laser-material interactions; Thin films (Laser-Assisted Processing by Pulsed Laser Deposition (PLD), Matrix Assisted Pulsed Laser Evaporation (MAPLE), CAD/CAM Rapid Prototyping by Matrix Assisted Pulsed Laser Evaporation Direct Write (MAPLE DW) & Reverse MAPLE - a novel chemical templating approach for controlled-release drug delivery systems). She has studied different biomaterials: pure/doped biomimetic hydroxyapatite; biopolymers (Polyethylene glycol (PEG); Polycaprolactone (PCL); chitosan; Poly(3-hydroxybutyric-acid-co-3-hydroxyvaleric-acid) (PHVB); poly(lactic-co-glycolic acid) (PLGA); polyaniline grafted lignin); Proteins: (Lysozyme, Silk Fibroin (SF)); Bacteria: (E. coli, S. aureus, B. subtilis, E. faecalis strains); Antimicrobial: (flavonoids; poly(1,3-bis-(p-carboxyphenoxy propane)-co-(sebacic anhydride)) /gentamicin sulfate; quercetin, resveratrol, lignin). She applied in her studies techniques for Material and Surface Investigation (e.g. FT-IR Spectrophotometry; Atomic Force Microscopy: AFM; Electron Microscopy: SEM, HRTEM; Electron Spectroscopy: XPS, AES). In special she focused on Biomedical Applications: Drug Delivery, Tissue Engineering, Faster Diagnosis and Treatment, Biofouling, Bio-chem sensors, Antimicrobial assays and 3D Printing. The originality of her results is confirmed by the publication of 19 ISI Indexed articles (5 – first author; 14 – co-author) in scientific journals of Q1, 1 book chapter; summing a Total citations of 265, Hirsh index: 10 - according to Scopus; Total citations: 250 (221 without self-citations): Hirsh = 9; according to Web of Science; Total citations: 315, Hirsh = 10 according to Google Scholar. (ResearcherID: I-7288-2016; ORCID 0000-0003-0539-4160). She is the project leader of a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2020-2273, within PNCDI III. She also has got favorable recognition by winning the national fellowship program L'Oréal—UNESCO "For Women in Science". Her international visibility is demonstrated by the involvement as a member of local organizing committee of 10th International Conference on Photoexcited Processes and Applications, as well as more than 75 participations at scientific communications (including 23 oral presentations and invited lectures) at National and International conferences, workshops and seminars in the related field. One note that during her research activity she won 1 Best Poster Awards and 2 Best Oral Presentations.

Composite drug delivery system based on Amorphous Calcium Phosphate as Efficient Antimicrobial Platforms

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We report on the successful deposition of antimicrobial chitosan-biomimetic nanocrystalline apatite – tetracycline thin films by Matrix Assisted Pulsed Laser Evaporation (MAPLE) using a KrF* excimer laser source ($\lambda = 248$ nm, ζ FWHM ≤ 25 ns). Typical FTIR spectra of the obtained thin films were found to be highly similar to the spectrum of the initial powders. Scanning electron microscopy have evidenced a typical morphology characteristic to the deposition technique, advantageous for medical application, the nanoscale roughness increasing with the chitosan concentration. We have evaluated the antibacterial properties of the thin films containing chitosan and tetracycline deposited by MAPLE on titanium samples, using as model organisms both the Gram-negative *E. coli* and Gram-positive *E. faecalis*. The biocompatibility of the obtained films deposited on Ti substrates was evaluated by in vitro tests on human bone osteosarcoma cells. These tests have revealed the morphology and cellular cycle of the cells growing on the obtained thin films. The results have demonstrated that the chitosan- biomimetic nanocrystalline apatite-tetracycline composite thin films have improved the bone formation and further facilitated the anchorage between the bone and prosthesis, thus validating the MAPLE efficiency.



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Barbara Freis is a PhD student at the University of Strasbourg in the IPCMS (Institut de Physique et de Chimie des Matériaux de Strasbourg) and at the university of Mons in Belgium under the supervision of professor Sylvie Bégin in Strasbourg and professor Sophie Laurent in Mons. Her PhD project concerns the synthesis of iron oxide nanoparticles for theranostic applications. She synthesizes iron oxide nanoparticles via thermal decomposition and tunes their size and shape by varying different parameters such as the temperature reaction, the heating rate, the nature of precursor, solvent and surfactant and their ratio. Then Barbara will perform a ligand exchange to have the nanoparticles coated with a dendron molecule which allows a good biocompatibility, a small hydrodynamic size and an anti-fouling effect. The next step is to graft different types and amounts of targeting ligand on the nanoparticles' surface to specifically target cancerous cells and test the therapeutic effect of the nanoparticles in vitro as well as in vivo. Different types of therapeutic modes are planned to be tested such as magnetic hyperthermia, photothermia, sonotherapy or protontherapy. The goal of her PhD is to assess the best nanoparticles design for multitherapy. Barbara was able to already show promising results for magnetic hyperthermia and photothermia for nanoparticles in suspension in water.

MASTERING SIZE FOR THE DESIGN OF INNOVATIVE THERANOSTIC IRON OXIDE BASED NANOPARTICLES ENSURING MULTIMODAL THERAPY

Barbara Freis^{1,2}, Francis Pertont¹, Celine Kiefer¹, Damien Mertz¹, Céline Henoumont², Christine Affolter-Zbaraszczuk³, Sebastien Harlepp³, Florent Meyer³, Sonia Furguele⁴, Fabrice Journe⁴, Sven Saussez⁴, Sophie Laurent^{2*}, Sylvie Bégin-Colin^{1*}

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In nanomedicine, the goal is to develop multimodal nanoparticles (NPs) to speed up targeted diagnosis, and increase its sensitivity, reliability and specificity for a better management of the disease. Combination of therapies is a way to increase the efficiency of anticancer treatment. Therefore, besides precision diagnosis, other challenges for personalized nanomedicine are to develop tools to be able to test quickly different treatments and to follow-up the effect(s) of the treatments by imaging.

Besides being excellent T2 contrast agents for MRI^[1], iron oxide NPs are promising as therapeutic agents by magnetic hyperthermia when correctly designed^[2]. To be a good heating agent, iron oxide NPs have to display a high magneto-cristalline anisotropy and ways to increase it are to tune the NPs size and shape^{[2][3][4]}. Iron oxide nanoparticles have also an interest for photothermal treatment as they express a good photothermal response to laser irradiation^[5]. Moreover, promising results shows that iron oxide NPs could be efficient sonosensitizers for anticancer treatment^[6]. Thus, other therapies such as sonotherapy and protontherapy should be tested with iron oxide NPs to study how they respond to them. The goal of this project is to develop iron oxides NPs with different sizes by the thermal decomposition method and by tuning synthesis parameters such as the reaction temperature, the heating rate and the

nature of surfactant ^{[2][3]}. Main difficulties were the reproducible synthesis of NPs with mean size higher than 12 nm, a homogeneous spinel composition and their dendronization. NPs with different sizes in the range 5-20 nm were thus synthesized and coated with dendron molecules. Their behaviors towards the different kinds of therapies were investigated both in suspension and in cells allowing to establish the optimal NPs design to combine therapies.

References:

- [1] Basly, B. et al. Effect of the nanoparticle synthesis method on dendronized iron oxides as MRI contrast agents. *Dalton Trans.* 42, 2146–2157 (2013).
- [2] Cotin, G. et al. Unravelling the Thermal Decomposition Parameters for The Synthesis of Anisotropic Iron Oxide Nanoparticles. *Nanomaterials* **8**, 881 (2018).
- [3] Baaziz, W. et al. Magnetic Iron Oxide Nanoparticles: Reproducible Tuning of the Size and Nanosized-Dependent Composition, Defects, and Spin Canting. *J. Phys. Chem. C* **118**, 3795–3810 (2014).
- [4] Cotin, G. et al. Evaluating the Critical Roles of Precursor Nature and Water Content When Tailoring Magnetic Nanoparticles for Specific Applications. *ACS Appl. Nano Mater.* **1**, 4306–4316 (2018).
- [5] Espinosa, A. et al. Magnetic (Hyper)Thermia or Photothermia? Progressive Comparison of Iron Oxide and Gold Nanoparticles Heating in Water, in Cells, and In Vivo. *Adv. Funct. Mater.* **28**, 1803660 (2018).
- [6] Ebrahimi Fard, A. et al., Synergistic effect of the combination of triethylene-glycol modified Fe₃O₄ nanoparticles and ultrasound wave on MCF-7 cells. *Journal of Magnetism and Magnetic Materials* **394**, 44–49 (2015).



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Dr.Eng. Alina Vladescu, has a B.S. in Materials Science and Engineering from the University Politehnica of Bucharest (2002) and an MS in Biomaterials from the Department of Bioengineering and Biotechnology, University Politehnica of Bucharest (2004). Her PhD however is in Materials Science from University Politehnica of Bucharest (2011). She works at National Institute for Optoelectronics, Department for Advanced Surface Processing and Analysis by Vacuum Technologies. She is also associate professor in Surface Engineering at University Politehnica of Bucharest. She is also affiliated as research scientist at National Research Tomsk Polytechnic University.

Expertise: • Functional coatings (metals, nitrides, carbides, oxides and oxynitrides) deposited by magnetron sputtering and cathodic arc techniques), especially for optics, optoelectronics, mechanical and tribological applications, but also with special properties, such as corrosion resistant and biomaterials. • Oxide thin films by electron gun evaporation technique, especially for optoelectronics applications and (again) for biomaterials. • Analysis and characterization of thin films using various spectroscopies (UV-Vis-NIR, EDS), X-ray diffraction, morphological, mechanical, anticorrosion and tribological characterization.

Guest Editor: *Frontiers in Materials* (2016-2017), *Composite Interfaces* (2016), *Coatings* (2019-2021).

Consequently, she has 123 technical publications and presentations, 10 patents, 3 books. Most of these articles have involved the surface biofunctionalization of metallic components of the biomedical devices by PVD deposition methods. In general, these articles have primarily proved that both PVD techniques (reactive magnetron sputtering and vacuum cathodic arc) represent a valuable choice for coating the metallic femoral heads, determining the increase of their service-life. Up to date she was involved in the investigation and assessment of various types of coatings, such as: nitrides, carbides, carbonitrides, oxynitrides or oxides, in mono and multilayered structures.

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Solution for decreasing of corrosion rate of MgCa alloy used in biomedical applications

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The growing implant market requires advanced Ti-based implants for long-term application, and for the newly engineered biodegradable Mg alloys with controllable dissolution rates for short-term applications. For this reason, Mg-alloys gain much more attention recently. Mg alloys are biodegradable material, but with too high corrosion rate and degradation occurs before the end of healing process. Moreover, during the corrosion, hydrogen released thereby causes pH increase of the surrounding tissue, inducing apoptosis and necrosis of tissue cells. For these reasons, it is a challenge to controlled degradation rate of Mg alloy and to provide sufficient time for the tissue to heal up to complete degradation of Mg implant.

The aim of the present paper is to investigate different types of CaP coatings as possible candidate for temporary implants made of MgCa1 alloy. The coatings were prepared by magnetron sputtering and micro-arc oxidation methods. The coatings were investigated in terms of microchemical, microstructural and mechanical properties, corrosion resistance in SBF at 37°C, as well as the biocompatibility with human cell line.

We acknowledge the support of the Romanian projects: no. COFUND-ERANET-RUS-PLUS-CoatDegraBac (no. 68/2018), within PNCDI III; Core Program-2020; no. 19PFE/2018 (PROINSTITUTIO).

8. INVITED PRESENTATION *Miguel Augusto PALHINHA CASTILLO*

11:30 (O.YIF.8)



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Miguel Castillo is a PhD student at the International Iberian Nanotechnology Laboratory (INL) in Braga, Portugal. He is working on natural photonic structures and their role on light absorption for photosynthesis. Using computer models, he simulates the photonic properties of these structures and estimate the consequences of light sensitive structural changes. From here, the biological advantages could be inferred, unveiling how photonics could play a role in one of the most fundamental and important natural processes: photosynthesis. A mimic is being developed for the natural photonic structure in order to reveal possible hidden properties. This research can inspire us to develop novel light sensitive photonic devices with tunable properties and develop the techniques for the fabrication of these devices. He has received and FCT fellowship supported by “Towards biomimetic photosynthetic photonics” project (POCI-01-0145-FEDER-031739) co-funded by FCT and COMPETE2020.

Martin Lopez-Garcia leads the Natural and Artificial Photonic Structures and Devices Research Group at INL. Martin’s main interests lie in the study of light-matter interactions in natural nanostructures and the development of biomimetic strategies for photonic applications. He is particularly interested in bioinspiration for energy harvesting. At INL he combines material science, biotechnology and advanced optical characterization for the development of cost-effective and sustainable photonic materials and devices.

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Castillo, Miguel A., William P. Wardley, and Martin Lopez-Garcia. "Light-Dependent Morphological Changes Can Tune Light Absorption in Iridescent Plant Chloroplasts: A Numerical Study Using Biologically Realistic Data." *ACS Photonics* 8.4 (2021): 1058-1068.

Tunable light absorption in iridescent nanostructured chloroplast

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Light has been used by nature as a source of energy for billions of years and chloroplasts play a crucial role harvesting this energy for high plants. Several species of deep shade plants show a specialized type of chloroplasts, named iridoplasts, which has evolved to present a well-defined arrangement of the photosynthetic tissue forming a periodic multilayer structure. This multilayer strongly reflects blue light and is an example of naturally occurring structural colour. Although the biological function of the iridoplast is still debated, experimental evidence suggests that the photonic structure might enhance light absorption and increase photosynthesis quantum yield [1].

Iridoplasts show a light sensitive behaviour, shifting between high reflectance and suppressed reflectance under low and high light conditions respectively. The mechanism by which iridoplasts adapt the photonic bandgap to different light conditions remains unknown but studies on non-photonic chloroplasts point towards compression and expansion of the membranes [2]. We use transfer matrix methods to calculate the change in the optical properties of the iridoplasts according to these documented light adaptations of the photosynthetic tissue. Our simulations include realistic structural data taken from the natural system. We find that, under high light conditions, the iridoplast reflection is redshifted and absorption enhancement is reduced comparing to low light conditions. These photonic properties are resilient to biologically realistic levels of disorder in the structure. This analysis is extended to another photonic structure containing chloroplast called bizonoplast. Similar results are concluded pointing towards similar properties in different plant species. Our results suggest that iridoplasts and bizonoplasts could tune their absorption and reflection by changing the photonic response of the multilayer according to the light environment.

This is an extraordinary case of photonic properties undertaking an important role in natural light harvesting. Understanding these natural systems can inspire us to develop new technologies for energy harvesting. In this communication we will also present preliminary result in producing biomimetic systems with similar optical properties to the ones found in iridoplast.

Work funded by “Towards biomimetic photosynthetic photonics” project (POCI-01-0145-FEDER-031739) co-funded by FCT and COMPETE2020.

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Dr. Monica Marini is a Senior Postdoc at the Department of Applied Science and Technology (DISAT) of the Polytechnic of Turin in Italy. Her research focuses on the mechanical and structural study of nucleic acids and their interactions with other biomolecules (e.g., Rad51 repair protein) and ligands such as chemotherapeutic compounds (Cisplatin), bis-intercalants (YOYO-1) and heavy metals (e.g. Nickel) to reveal their connection to diagnosis and disease. To reach this goal, conventional bio-molecular, -chemical and -physical tools are combined with microfabrication, high-resolution TEM imaging and diffraction, Raman spectroscopy, and Laser Doppler Vibrometer.

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DNA-Superhydrophobic surfaces platforms for sensing and structural studies

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Recently, we used super-hydrophobic surfaces (SHS) to obtain suspended DNA molecules and bundles with a simplified physiological-compatible preparation procedure. A droplet of a saline solution containing nucleic acids is deposited over the SHS and at room temperature it spontaneously dehydrates and retracts from one pillar to the next in line without collapsing. The DNA molecules linked to the top of a pillar are pulled, following the drop movement: with this method we obtained free-standing self-assembled DNA fibers, studied by HRTEM [1,2], Raman Spectroscopy [3,4] and Laser Doppler Vibrometer [5]. The DNA-SHS platform allows characterizing native nucleic acids molecules and the variations to the pristine conditions as the ones occurring after the interaction with ligands such as intercalants, chemotherapeutic drugs and proteins by using different techniques and achieving quantitative information. This approach can find its application in medical-oriented research for personalized drugs administration (e.g., CisPt-DNA adducts), food safety (e.g., mycotoxins-DNA adducts), and the study of environmental pollutants effects on the double helix.



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Sergey Turishchev is Associate Professor at the Solid State Physics and Nanostructure Dept, Head and Leading Researcher of the Electronic Structure of Solids Laboratory at the Physics Faculty of the Voronezh State University, Russia. Scientific and Educational activities are placed at the intersection between solid state physics, atomic and electronic structure of solids and nanosystems, X-ray and electron spectromicroscopy, synchrotron radiation studies, functional nanomaterials including bio-hybrid. He is co-authored of more than 70 publications in scientific journals (h-index 12). Regular speaker at E-MRS Spring Meetings symposia range since 2007. He has headed more than 20 scientific projects including international level. Since 2002 conducting experiments with the use of synchrotron radiation for more than 30 beamtime projects headed at a range of large scale facilities. Scientific group includes 10 young scientists at PhD or PhD student level.

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.

Qun MA

Towards Explicit Regulating-Ion-Transport: Nanochannels with only Function-Elements at Outer-Surface

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Function elements (FE) are vital components of nanochannel-systems for artificially regulating ion transport. Conventionally, the FE at inner wall (FEIW) of nanochannel-systems are of concern owing to their recognized effect on the compression of ionic passageways. However, their properties are inexplicit or generally presumed from the properties of the FE at outer surface (FEOS), which will bring potential errors. Here, we show that the FEOS independently regulate ion transport in a nanochannel-system without FEIW. The numerical simulations, assigned the measured parameters of FEOS to the Poisson and Nernst-Planck (PNP) equations, are well fitted with the experiments, indicating the generally explicit regulating-ion-transport accomplished by FEOS without FEIW. Meanwhile, the FEOS fulfill the key features of the pervious nanochannel systems on regulating-ion-transport in osmotic energy conversion devices and biosensors, and show advantages to (1) promote power density through concentrating FE at outer surface, bringing increase of ionic selectivity but no obvious change in internal resistance; (2) accommodate probes or targets with size beyond the diameter of nanochannels. Nanochannel-systems with only FEOS of explicit properties provide a quantitative platform for studying substrate transport phenomena through nanoconfined space, including nanopores, nanochannels, nanopipettes, porous membranes and two-dimensional channels.

Micaela MATTA**Eumelanin: a biocompatible mixed conductor**

Micaela Matta, Alessandro Troisi

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Organic bioelectronics is an interdisciplinary research area which involves the development of polymer semiconductors for nanomedicine and healthcare applications, such as wearable, implantable, diagnostic or sensing devices.¹ Polymers are ideal candidates for bioelectronics, as their mechanical, physical and chemical properties can be tailored to match those of cellular tissues. A possible way to obtain biocompatible materials for bioelectronics is to exploit naturally occurring compounds, either alone or in composite materials. Eumelanin is an amorphous insoluble pigment present in both mammals and invertebrates. Eumelanin consists of amorphous aggregates of DHI (5,6-dihydroxyindole) and DHICA (5,6-dihydroxyindole-2-carboxylic acid) oligomers, interacting via π -stacking and hydrogen bonding. Synthetic melanins are usually obtained using either DHICA or DHI and present a lower degree of structural disorder; they are being investigated for energy storage/production² and as composite materials for biomedical applications.³ We present a systematic study of the electronic structure and conformational space of DHICA oligomers, characterized by a linear polymeric structure and strong antioxidant properties. Our computational insight not only fits well within existing experimental evidence, but can also predict the charge transport landscape in the bulk polymer.² We then use molecular dynamics simulations to study the amorphous structures formed by this material, and investigate its aggregation-dependent excited state properties. Finally, we describe our approach towards the simulation of realistic DHI melanin aggregates using a combination of experimental evidence, statistics and molecular dynamics.

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Matthew Wei Ming Tan is a PhD student at Nanyang Technological University, School of Material Science and Engineering and is supervised by Professor Lee Pooi See. His research interests include smart materials, flexible/stretchable electronics, and soft robotics. Particularly, he synthesizes novel elastomers that are applied towards dielectric elastomer actuators (DEAs), at which these soft actuators achieve improved actuation performances and are imparted with unique features such as self-healing abilities and high toughness. Based on his work on soft actuators, he was recently awarded with the 2020-2021 Travel Award sponsored by the journal *Actuators*. Finally, he is a first author of two published articles, coauthor of two review articles and three more in preparation.

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Designing Highly Stretchable, Tough and Self-healing Supramolecular Elastomers for Artificial Muscles

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Dielectric elastomer actuators (DEAs) are often coined as artificial muscles for soft robotic systems. Moreover, when utilized in combination with self-healing materials these artificial muscles take a giant leap towards being like its biological counterparts. With self-healing capabilities, DEAs can "heal" from external damages similar to the body that closes off a wound for recovery. However, while promising for soft robotics, current self-healing elastomers used are lacking intrinsic toughness, causing the actuator to become susceptible to external damages in the first place. In this work, we address this by designing a carboxyl polyurethane (COOH-PU) with high toughness, absorbing energy without fractures. COOH-PU possesses multiple hydrogen bond functionalities to allow dynamic supramolecular interactions to reassociate upon damage for self-healing. However, the main challenge of designing tough self-healing elastomers for DEAs is attaining low elastic moduli for high actuation performances. To overcome this, soft segment of COOH-PU was tuned in accordance to molecular weight, in order for strain hardening to take effect at higher strains. As such, the elastic modulus was drastically reduced from 22.6 to 2.6 MPa, reaching values similar to soft tissues. Concurrently, high toughness of 283.8 MJ m⁻³ is attained, exceeding the toughness of armored scales of animals such as the armadillos. Furthermore, carboxyl groups provide high dielectric constant critical for achieving high actuation performances. Therefore, through these molecular designs from COOH-PU, artificial muscles can be tough and robust, achieve high actuation performances and even prolong their operations from self-healing effects.

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Kiefer Ramberg

Kiefer completed a BSc in Biopharmaceutical Chemistry at NUI Galway, Ireland, graduating with a 1st class honours degree. During his BSc, Kiefer spent time in industry and also carried out a short research project in the lab of Prof Peter Crowley, which ultimately led to him becoming a PhD candidate in 2016. Having been awarded an NUI Travelling Studentship, one of Ireland's oldest sources of postgraduate funding, Kiefer spent time at the CERM NMR Facility in Florence, Italy working on a Horizon2020-funded project on PEGylated proteins. Kiefer's research focuses on protein recognition and assembly mediated by synthetic macrocycles. His latest work on the fabrication of porous protein-macrocycle frameworks has been published in *J. Am. Chem. Soc.* in 2021. Kiefer has presented his work at several international meetings, including the International Symposium on Macrocylic and Supramolecular Chemistry (ISMSC).

Prof. Peter B. Crowley

Peter Crowley is a graduate of University College Dublin and Leiden University. In 2008, he joined NUI Galway and established his laboratory in the field of biosupramolecular chemistry. He was promoted in 2014 to Senior Lecturer and in 2017 to Personal Professor. Since 2020, he is a topic editor at *Crystal Growth & Design*. Current research is focused on macrocycle-directed assembly of protein frameworks.

Publication List

1. **Ramberg KO**, Engilberge S, Skorek, T, and Crowley PB. Facile Fabrication of Protein-Macrocycle Frameworks. *J. Am. Chem. Soc.* 2021, *As soon as publishable*.
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Facile Fabrication of Protein – Macrocycle Frameworks

Kiefer O. Ramberg,^a Sylvain Engilberge,^{a,b} Tomasz Skorek,^a and Peter B. Crowley^a

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Precisely defined protein aggregates as exemplified by crystals have applications in functional materials.¹ Consequently, engineered protein assembly is a rapidly growing field. Strategies involving protein assembly via supramolecular ligands are gaining momentum.² Anionic calix[n]arenes are particularly useful scaffolds that can mould to cationic protein surfaces and consequently induce oligomerisation.^{3,4} Here, we describe the manufacture of protein-calixarene composites *via* co-crystallization of sulfonato-calix[8]arene (**sclx8**) with the symmetric and “neutral” protein RSL. Co-crystallization occurred across a wide range of conditions and protein charge states, from pH 2.2-9.5, resulting in three crystal forms. Cationization of the protein surface at pH ~4 drives complexation and yielded two types of porous protein frameworks. Calixarene-masked proteins act as nodes within the frameworks, displaying octahedral-type coordination in one case. The other framework forms millimetre-scale crystals within hours at pH 4, without the need for precipitants or specialised equipment. NMR experiments revealed macrocycle-modulated side chain p*K*_a values, consistent with pH-triggered assembly. The same type of framework was generated with an arginine-enriched RSL variant at high pH. Finally, in addition to protein framework assembly, **sclx8** can be used for *de novo* structure determination via sulfur SAD.

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Hayeon KIM

Supramolecular antifreezing peptide nanoagents for cellular cryopreservation

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Cryopreservation is critical factor in a fields of biochemical, pharmaceutical, biotechnological, and food industries, when it comes to storing cells, tissues, proteins, drugs, and foods. Antifreeze proteins (AFPs) have attracted huge interest with their cryopreservation activity originated from ice recrystallization inhibition or thermal hysteresis effects, which prevents organisms from freezing at the subzero environment. It is still challenging to develop new cryoprotectants mimicking natural AFPs for practical use due to the lack of understanding of structure-antifreezing activity relationship. The commercially available antifreezing agents show potential cytotoxicity to be applied for a biomedical field. Here, the self-assembled peptide nanoagents mimicking the AFPs were rationally designed by supramolecular chemistry to enhance both antifreeze activity and biocompatibility. The various nanostructures of the peptide nanoagents, changed by the hydrophobicity and hydrophilicity of periodically arranged antifreezing moieties, affect ice binding and resultant ice growth inhibition. Then it was confirmed that the survive rate of frozen-thawed stem and germ cells were increased after cryopreservation of peptide nanoagents and the revitalization of them were evaluated. This research could provide a useful strategy for manufacturing a cryopreservation agents with high performance through supramolecular chemistry and figuring out the mechanism of how AFPs affects cellular cryopreservation.

*INVITED PRESENTERS: The 7en minutes Report on Frontier Research
(14.00 h – 17.00 h)*

17. Monica Marini

14:00 (O.YIF.17)



Dr. **Monica Marini**, Postdoctoral Fellow
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Fields of Interest and Expertise:

Dr. Monica Marini is a Senior Postdoc at the Department of Applied Science and Technology (DISAT) of the Polytechnic of Turin in Italy. Her research focuses on the mechanical and structural study of nucleic acids and their interactions with other biomolecules (e.g., Rad51 repair protein) and ligands such as chemotherapeutic compounds (Cisplatin), bis-intercalants (YOYO-1) and heavy metals (e.g. Nickel) to reveal their connection to diagnosis and disease. To reach this goal, conventional bio -molecular, -chemical and -physical tools are combined with microfabrication, high-resolution TEM imaging and diffraction, Raman spectroscopy, and Laser Doppler Vibrometer.

Selected publications:

- [1] P. Zhang, M. Moretti, M. Allione, Y. Tian, J. Ordonez-Loza, D. Altamura, C. Giannini, B. Torre, G. Das, E. Li, S. T. Thoroddsen, S. M. Sarathy, I. Autiero, A. Giugni, F. Gentile, N. Malara, **M. Marini** & E. Di Fabrizio. *Communications biology* **2020**, 3, 457.
- [2] S. Stassi*; **M. Marini***; M. Allione; S. Lopatin; D. Marson; E. Laurini; S. Pricl; C.F. Pirri; C. Ricciardi; E. Di Fabrizio, *Nat. Commun.* **2019**, 10, 1690.
- [3] **M. Marini**; M. Allione; S. Lopatin; M. Moretti; A. Giugni; B. Torre; E. di Fabrizio, *Microelectron. Eng.* **2018**, 187–188, 39–42.
- [4] **M. Marini***; T. Limongi*; A. Falqui; A. Genovese; M. Allione; M. Moretti; S. Lopatin; L. Tirinato; G. Das; B. Torre; A. Giugni; F. Cesca; F. Benfenati; E. Di Fabrizio, *Nanoscale*. **2017**.
- [5] **M. Marini**; M. Allione; B. Torre; M. Moretti; T. Limongi; L. Tirinato; A. Giugni; G. Das; E. di Fabrizio, *Microelectron. Eng.* **2017**, 175, 38–42.
- [6] **M. Marini**; A. Falqui; M. Moretti; T. Limongi; M. Allione; A. Genovese; S. Lopatin; L. Tirinato; G. Das; B. Torre; A. Giugni; F. Gentile; P. Candeloro; E. Di Fabrizio, *Sci. Adv.* **2015**, 1, e1500734–e1500734.
- [7] **M. Marini**; G. Das; R. La Rocca; F. Gentile; T. Limongi; S. Santoriello; A. Scarpellini; E. Di Fabrizio, *Microelectron. Eng.* **2014**, 119, 151–154.

DNA/LIGANDS STRUCTURAL STUDY

Monica Marini,¹ S. Stassi,¹ M. Allione,² F. Legittimo,¹ B. Torre,¹ A. Giugni,³ M. Moretti,⁴ C.F. Pirri,^{1,2} C. Ricciardi,¹ E. Di Fabrizio¹

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Recently we obtained free-standing self-assembled biomolecules fibers, by using a physiological compatible preparation and super-hydrophobic surfaces (SHS). A droplet of the biomolecule solution is deposited over the SHS. At room temperature, the water in solution evaporates: the droplet decreases in volume and moves from one pillar to the next. With this method the molecules in solution are pulled and linked between micro-pillars. We suspended DNA, DNA/ligands, and cell membranes that were characterized by EM, Raman Spectroscopy and Laser Doppler Vibrometer. The DNA fibers allowed us obtaining background-free TEM direct images and measuring DNA bases and backbone without the use of contrast agents, with a resolution of 1.5 Å. TEM diffraction confirmed the quantities measured. Raman spectroscopy data expanded the EM data with structural/chemical information on DNA monomers, conformation and fluctuations related to the environment. DNA bundles were also used as ultrasensitive mechanical resonators to detect and study deviations to the native form, by administering intercalants and the chemotherapy cisplatin at increasing concentration. Alteration to sizes and Young's modulus were successfully quantified. Overall, the results show that our approach can be applied to medical-oriented developments such as personalized drugs administration (e.g., CisPt-DNA adducts), food safety (e.g., mycotoxins-DNA adducts), and the study of environmental pollutants effects on the double helix.

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Nanostructured and Functionalized Microcantilevers for Fast Detection of Vapors

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Chemical Warfare Agents (CWA) and explosives detection with a high sensitivity and selectivity is crucial due to the growing threats from terrorist organizations to human health. Fast, selective and sensitive sensing methods are required to reduce the threat against CWAs. Microgravimetric sensor platforms with chemo or physico-selective interfaces offer an ideal solution to the previous drawbacks. We developed a bio-inspired nanostructured and functionalized cantilever for the detection of ultralow concentrations of explosives and simulants (DMMP (DiMethyl MethylPhosphonate) of CWA with different materials (TiO₂, ZnO, CuO and Cu(OH)₂) and morphologies (nanotubes or nanorods) in order to increase the surface area of adsorption and the limit of detection. This strategy of nanostructuring and functionalization promises significant improvements over existing sensors and for the next generation of cantilevers.



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PhD student Anastas A. Romansky studies under supervision of Prof. Volodymyr L. Karbivskii at G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine. He has obtained his Bachelor Degree in Physics in 2017 at National Aviation University, Master Degree in 2019 at Kyiv Academic University. His main scientific interests are: nanomaterials, electronic structure.

Volodymyr L. Karbivskii is director of the SPM&RS-Centre and head of Department of Nanostructures Physics of G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, Doctor of Physics, professor, laureate of State prize in Ukraine in the field of physics and technology (2015). In 1987 he graduated from the Faculty of Physics of the Taras Shevchenko National University of Kyiv. In 1990 he defended his Ph.D. thesis, in 2005 - his doctoral dissertation. In 2004 - 2009, the head of the direction "Biosystems and bionanomaterials, artificial biomineralization of nanomaterials, application of nanomaterials in biology and medicine" of the program of the N.A.S. of Ukraine "Nanostructural systems, nanomaterials, nanotechnologies". Member of the section "Physics of Nanostructured Systems" of the Interdepartmental Scientific Council on the Problem of Solid-State Physics. Scientific interests are concentrated on nanobiotechnologies of structures of biomedical and ecological applications, physics of disordered systems and surface phenomena physics.

Lyubov I. Karbivska is an employee of Department of Nanostructures Physics. In 2005 she graduated from the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". She defended her Ph.D. thesis in 2009, her doctoral dissertation – in 2019. [Her main scientific interests are carbon nanomaterials and nanotechnology.](#)

The influence of synthesis conditions on the electronic structure and structural characteristics of bioactive ceramics and glass

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Previously, we developed samples of biocompatible composite based on calcium phosphates – "Syntekost" (synthetic bone). The aim of this work is to optimize the properties of bioactive materials for bone tissue recovery – ensuring their oncoprotective and anti-inflammatory properties. At various temperature conditions, a number of inorganic materials were synthesized: calcium phosphate ceramics, glasses and sitalls, as well as composites based on nanodispersed calcium hydroxyapatite. The effect of synthesis temperature conditions on the structure and properties of the obtained materials is investigated. Doping of a number of samples with bioactive elements was carried out with the aim of their functionalization. Samples of conductive bioactive nanocomposites based on nanodispersed apatite and nanodispersed graphite were obtained, and their properties were studied by electrophysical methods. An analysis of the XPS data of the obtained samples showed that, depending on the conditions of glass synthesis – melt cooling rate, temperature regime, and glass doping, the binding energy of the constituent elements changes. The temperature conditions of the process for producing such materials were optimized. The relative fraction of bioactive calcium phosphates and their crystallinity correlate with synthesis conditions, in particular – temperature regime. The XPS data for the fused glass sample indicate the presence of CaSiO₃ and Mg₂SiO₄, which are associated with bio-sitalls.



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Alina Sharova obtained M.Sc. degree in Laser Physics at National Research Nuclear University MEPhI (Moscow, Russia) in 2018. From 2016 to 2018 she was carrying out research in biophotonics (emphasis on phototheranostics and biospectroscopy) at General Physics Institute of the Russian Academy of Sciences (Moscow, Russia). At that time, she interned at Princess Margaret Cancer Centre (Toronto, Ontario, Canada). Now Alina is a PhD student working on Edible electronics at the Center for Nano Science and Technology@PoliMi (CNST) of the Istituto Italiano di Tecnologia (IIT, Milan, Italy) in the Printed and Molecular Electronics group, led by Dr. Mario Caironi. Her current research interests focus on bio and nanotechnology, food science and electronics for the healthcare.

Dr. Mario Caironi obtained his Ph.D. in Information Technology with honours at Politecnico di Milano (Milan, Italy). In 2007 he joined the group of Prof. Sirringhaus at the Cavendish Lab. (Cambridge, UK) as a post-doc, working on high resolution printing of downscaled organic transistors and circuits. In 2010 he was appointed as Team Leader at the Center for Nano Science and Technology@PoliMi (CNST) of the Istituto Italiano di Tecnologia (IIT, Milan, Italy). In 2014 he entered the tenure track at the same institution, obtaining tenure in 2019. He is currently interested in solution based high resolution printing techniques for micro-electronic, optoelectronic and thermoelectrics devices, in the device physics of organic semiconductors-based field-effect transistors, in biomedical and/or implantable sensors and electronics for the healthcare.

Towards edible electronic devices: low voltage honey-gated organic transistors and circuits

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The use of natural and bioinspired materials is an emerging key approach towards development of new-generation safe technology. Going beyond the traditional concept of electronic devices, we convey the idea of making electronics edible. This unconventional approach exploits the electronic properties of natural and food-based materials for developing ingestible functional devices. Critical biomedical, pharmaceutical, and food industry applications are targeted by the proposed field. In this framework, we explore the potential of cost-effective and edible substance, honey, to be used as electrolytic gate viscous dielectric. Honey-gated organic field effect transistors (OFETs) based on both n & p type semiconductors are fabricated. A distinctive feature of these transistors is their long-term stability, reproducibility and low voltage $< 1V$ operation in air. Devices exhibit forward-looking electronic performances, notably, electron and hole mobility–capacitance product of $3.5 \times 10^{-3} \mu\text{F}/\text{Vs}$ and $23 \times 10^{-3} \mu\text{F}/\text{Vs}$, respectively, surpassing ones of the previously reported water-gated OFETs. Furthermore, the observed devices responsivity to humidity provides promising opportunities for sensing applications. We then demonstrate, for the first time, the implementation of honey-based integrated circuits: inverting logic gate and ring oscillator. Lastly, honey-gated OFETs are fabricated on edible flexible tattoo-paper substrate that acts as a versatile platform for organic edible electronics [1].

[1] Giorgio E. Bonacchini, Caterina Bossio, Francesco Greco, Virgilio Mattoli, Yun-Hi Kim, Guglielmo Lanzani, and Mario Caironi, Tattoo-Paper Transfer as a Versatile Platform for All-Printed Organic Edible Electronics, *Advanced Materials* 30 (14): 1706091, 2018



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David Beke is currently a research fellow at the Wigner Research Centre for Physics and the Budapest University of Technology and Economics. His work focuses on ultrasmall nanoparticles and optically active defects in solids. Small clusters often have surface-dependent and size-dependent optical properties below 10 nm, allowing a wide variety of tuning and exploring new physics. Point defect in solids, on the other hand, are atom-like structures can have Magneto-optical properties influencing the behavior of the host material. The combination of the two can help new developments and discoveries in therapeutics, imaging, diagnostics, and quantum-technology.

David Beke graduated at the Budapest University of Technology and Economics as a Chemical engineer and got his Ph.D. in the same institute in Chemistry. He won the Graduate Student Award of the European Materials Society, the Budapest University of Technology Research Grant, and the Hungarian Academy of Sciences Early Career Researcher Award. His research was supported by the National Excellence Program two times and the National Talent program three times. David is currently supported by the János Bolyai Research Fellowship of the Hungarian Academy of Sciences.

Enhancement of Red X-Ray Excited Luminescence of Chromium Doped Zinc Gallate by Ultrasmall Silicon Carbide Nanocrystals

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X-ray activated near-infrared luminescence nanoparticles are considered as new alternative optical probes in life sciences. This is due to being free of autofluorescence and the excitation and emission possess a high penetrable nature in-vivo. Chromium-doped zinc gallate nanoparticles proved to have long-lasting persistent luminescence upon X-ray, UV or even visible light activation, allowing the excitation and emission to be separated in time. This paves the way for new types of imaging and even enhanced photodynamic therapy. The photoluminescence quantum yield, however, depends strongly on the dopant concentration and codoping for increased emission efficiency which is challenging because of the enhanced difficulty of handling dopants in the few-ppm-range. Here we report silicon carbide quantum dot sensitization of chromium-doped zinc gallate nanoparticles with enhanced near infrared radiation upon X-ray excitation. Using ultra-small SiC nanocrystals as a seed enables low-temperature hydrothermal synthesis with good crystal quality and optical properties without the need of post-annealing. SiC sufficiently decreases the escape probability and increases the emission efficiency by orders of magnitude upon X-ray excitation.



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Alesh Kumar is Ph.D. student of National Institute of Technology supervised by Asst. Prof. Dr. C.R.Mariappan. His research interests are therapeutic ions containing bioactive materials for bone tissue engineering. In particular, he developed different therapeutic ion doped mesoporous bioactive material for bone implants. He has six papers in reputed journals. He is recipient of MHRD India Senior research fellowship. He is also involved in characterization of materials for energy devices.

Dr. **Amilan Jose D.** received his Ph.D. from Central Salt and Marine Chemicals Research Institute (CSIRLab) in Bhavnagar, Gujarat, India and completed his postdoctoral research at the University of Regensburg in Germany, University of Jena in Germany, University of Bielefeld in Germany, ICIQ, Tarragona Spain. and UJF, France. His main research interest focuses on Functional Nanomaterials for the sensors, drug delivery, and Energy storage, Sensor for biologically important species and Supramolecular Chemistry.

Silver containing mesoporous bioactive glass ceramics nanoparticles as multifunctional agent for Bone tissue engineering

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Bioactive materials are designed to interface with biological systems to treat, augment, or replace any tissue, organ, or function of the body. Among the different types of biomaterials, the mesoporous bioactive glass-ceramics (MBCs) are containing control amount of different ions with the aim of different activity like as antibacterial, osteogenesis and angiogenesis. Here we report the synthesis, characterization and bioactivity of different composition of silver containing MBCs. Bioactive glass-ceramics were synthesized by used CTAB. The introduction of Ag₂O into the MBCs is intended to minimize the risk of microbial contamination through the potential antimicrobial activity of the leaching silver ions. The prepared samples were characterized by small angle X-ray scattering (SAXS), Fourier Transform infrared (FTIR) spectroscopy and high resolution transmission electron microscopy (HR-TEM). The SAXS patterns of samples show the agglomerates of ~15.3 nm average size with high polydispersity in size and size of the agglomerates varies from 2-40 nm range. FT-IR spectra show possible stretching and bending vibration modes of silicate and borate groups. HR-TEM confirms the mesoporous nature of MBCs. Bioactivity of MBCs was investigated by immersion of samples in simulated body fluid (SBF) at different time point followed by XRD and FTIR studies. The XRD patterns clearly show diffraction peaks of bone-like hydroxyapatite after immersion in DMEM. Silver-MBCs nanoparticles and there ionic dissolution extracts exhibited antibacterial effect against both positive and negative bacteria. Keywords: Bioactive glass-ceramics, Biocompatibility, Hydroxyapatite



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Development of an innovative fiber optic - surface plasmon resonance (FO-SPR) sensor for food and environmental monitoring

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Fiber Optic – Surface Plasmon Resonance (FO-SPR) technology has been recognized as a remarkable optical sensing tool in various fields of medicine, agro-food industry and environmental science, as it provides efficient characterization and real-time quantification of various chemical, physical and biological entities. For the FO-SPR sensors fabrication, noble metals (i.e. gold or silver) are used. Beyond these overused plasmonic materials, there are limited studies demonstrating the employment of other metals such as platinum (Pt) for SPR sensing applications. In this work, results on the fabrication and characterization of a SPR sensor using coatings of Pt and polyaniline (PANi) polymer layers over an unclad FO core were reported. The thin Pt layer was deposited using a magnetron sputtering technique, while the sensitive PANi layer was synthesized using an electroless polymerization approach. The PANi based FO-SPR sensor was morphologically characterized and evaluated for two applications: (i) pH monitoring and (ii) p-Nitrophenol pesticide detection. The obtained results showed that the FO-SPR pH sensor exhibited a fast and linear response in either acid or alkali solution (pH operational range 1 to 14). Moreover, the p-Nitrophenol limit of detection was found to be in the low pM concentrations range. Not in the least, the Pt-coated FO-SPR sensor was successfully applied also for Ara h1 peanut allergen detection using aptamers as bioreceptors. Concluding, this work represents a step forward in the fabrication of FO-SPR sensors, not only with improved performance, but also with extended functionality.



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Fabrication of Alumina Membrane Coated Titanium Implants for Effective Osteointegration

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In order to obtain an effective integration between an implant and a bone, implant surfaces should have similar properties with bone tissue surfaces. Especially mimicry of the chemical, mechanical and topographic properties of the implant to the bone is crucial for fast and effective osseointegration. Titanium based biomaterials are more preferred in clinical use and there are studies of coating these implants with oxide layers that has chemical/nanotopographic properties stimulating cell interactions for enhanced osseointegration. There are low success rates of current implantations especially in craniofacial implant applications which are large and vital zones and the oxide layer coating increases bone-implant integration providing long-lasting implants without requiring revision surgery. Our aim in this study is to examine bone-cell behavior on titanium implants with aluminum oxide layer (AAO) on effective osseointegration potential in deformation of large zones with difficult spontaneous healing. In our study, aluminum layer coated titanium surfaces were anodized in sulfuric, phosphoric and oxalic acid which are the most common used AAO anodization electrolytes. After morphologic, chemical and mechanical tests on AAO coated Ti substrates, viability, adhesion and mineralization of adult bone cells on these substrates were analyzed. Besides with Atomic Layer Deposition (ALD) as a sensitive and conformal technique, these surfaces were coated with pure alumina (5 nm) thus cell studies were performed on ALD-coated nano porous oxide layers with suppressed ionic content too. Lastly in order to investigate the effect of the topography on the cell behavior, flat non-porous alumina layers on silicon wafers formed by ALD were compared with the porous ones. Cell viability ratio was similar between anodized surfaces, but pure alumina coated titanium and anodized surfaces showed higher viability ratio compared to bare titanium and bare anodized ones. Alumina coated titanium surfaces which are anodized in phosphoric acid, showed significantly different mineralization ratios after 21 days over other bare titanium and titanium surfaces which anodized in other electrolytes. Bare titanium was the second surface that had highest mineralization ratio. Otherwise, titanium which is anodized in oxalic acid electrolyte demonstrated lowest mineralization. No significant difference was shown between bare titanium and anodized surfaces except AAO titanium surface anodized in phosphoric acid. Currently, osteogenic activities of these cells on genetic level are investigated by quantitative real time polymerase chain reaction (qRT-PCR) analysis results of RUNX-2, VEGF, OPG and OPN genes. Also as a result of the activities of the genes mentioned before, Western Blot will be used for protein detection. The project is supported by The Scientific and Technological Research Council of Turkey.

Keywords— alumina, craniofacial implant, MG-63 cell line, osseointegration, oxalic acid, phosphoric acid, sulphuric acid, titanium

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E-mail: wei.yu@kuleuven.be**Hybrid hydrogel matrices for remote cell actuation
and localized temperature monitoring**

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In living tissues, cells are supported by 3D extracellular matrices (ECM) that control and supports the cellular functions (i.e., adhesion, differentiation, migration, polarization etc.). A large variety of engineered nanomaterials, including nanofibers and hydrogels, with 2D or 3D architectures have been engineered to mimic the biochemical and mechanical properties present in natural ECMs. Moreover, a wide range of functional nanomaterials can be added to tissue culture scaffolds to impart them with remotely controllable, localized cellular cueing properties. Among potential scaffold material candidates, hydrogels were widely used to mimic many important functions of extracellular matrices found in living tissues [1, 2]. In this work, we construct hybrid cellular matrices based on hydrogels incorporating, fluorescent probes and plasmonic gold nanoparticles (AuNPs). Plasmonic nanoparticles allow for light-addressable photothermal [3, 4] and electrical stimulation functionalities to control cellular behavior. Localized heating is implemented in hydrogels by functionalizing them with gold nanorods (GNR) with LSPR peak around 785 nm, while the local temperature is reported by Rhodamine B (RhB)-loaded silica particles or quantum dots. We discuss in detail the necessary requirements, limitations and solutions to obtain reliable 2 and 3D temperature measurements in cellular matrices based on these nanoprobles. With the help of the developed experimental framework, we demonstrate that NIR illumination combined with AuNR leads to local temperature gradients in 3D hydrogels that can exceed 10 degrees in amplitude, with no detrimental effect on the network structure. Finally, SH-SY5Y neuroblastoma cells are cultured in the hybrid hydrogels and monitored by optical microscopy and metabolic assays. Satisfactory cellular viability with respect to hydrogel samples and positive preliminary results on cell actuation in 2 and 3D upon localized heating demonstrate excellent prospects for using the hybrid hydrogel scaffolds for localized cellular stimulation in both 2D and 3D cultures.

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Now, **Invited Organizer/Chair and Invited Presenter Young Investigator Forum at The Symposium O, The E-MRS Spring Virtual Conference 2021.**

Kaoru Toko is Associated Professor of Applied Physics at University of Tsukuba, Japan. He obtained his Ph.D degree in Engineering at Kyushu University in 2011 and joined the faculty at University of Tsukuba. His research interests include solar cells, thin film transistors, thermoelectrics, and rechargeable batteries based on inorganic semiconductors. For the remarkable achievements regarding these studies, he has won more than 10 awards and has published over 200 peer-reviewed papers with approximately 4000 citations in total.

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1. T. Imajo, K. Toko, R. Takabe, N. Saito, N. Yoshizawa, and T. Suemasu, Fabrication of SrGe₂ thin films on Ge (100), (110), and (111) substrates, *Nanoscale Research Letters* **13**, 22 (2018).
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Possibility of Ge-based materials for flexible thin-film transistors

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For the advancement of the ubiquitous computing society, it is desirable to develop wearable devices allowing information to be exchanged at all times and in all places. In particular, flexible devices equipped with superior computing performance over Si integrated circuits will be innovative devices such as multi-functional display. Group IV semiconductor Ge has a higher mobility than Si and is expected to be applied to high-speed devices. It also has a low crystallization temperature and can be synthesized directly onto flexible plastics under the heatproof temperature. Based on this background, intensive research has been conducted on the low-temperature synthesis of polycrystalline Ge (poly-Ge) thin films on insulators. However, although various methods have been investigated, the grain size was small ($< 1 \mu\text{m}$) and the films quality were too poor for practical use. We are focusing on solid phase crystallization (SPC), which is a simple method to directly form poly-Ge thin films on insulating substrates at low temperatures. Recently, in SPC, we found that the densification of an amorphous Ge precursor and adding Sn atoms in the precursor dramatically enlarged the grain size ($> 1 \mu\text{m}$) and improved hole mobility ($> 300 \text{ cm}^2/\text{Vs}$) [1,2]. The insertion of a GeO_2 underlayer further improved the hole mobility of Ge [3]. In this study, we investigated the detailed effect of the GeO_2 underlayer on the SPC-Ge, elucidated the mobility enhancement mechanism, and applied this method onto plastic substrate. As a result, we found that a small amount of oxygen diffusion from GeO_2 into Ge contributes to the grain size enlargement ($> 10 \mu\text{m}$) and defect compensation. Moreover, due to less thermal expansion difference, the SPC-Ge on a plastic substrate exhibited higher hole mobility than that of bulk Si [4]. This result means that single-crystal wafers are no longer necessary for a high-mobility semiconductor thin film. Besides, the resulting hole mobility $690 \text{ cm}^2/\text{Vs}$ is the highest value to date among those of semiconductor layers directly formed on insulators at low temperatures. This achievement will give a way to realize advanced electronic and optical devices simultaneously allowing for high performance, inexpensiveness, and flexibility. [1] K. Toko *et al.*, *Sci. Rep.* **7**, 16981 (2017). [2] K. Moto *et al.*, *Scientific Reports* **8**, 14832 (2018). [3] T. Imajo *et al.*, *Applied Physics Express* **12**, 015508 (2019). [4] J. C. Irvin and S. M. Sze, *Solid-State Electron* **11**, 599 (1968).



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1. [T. Nishida](#), K. Moto, N. Saitoh, N. Yoshizawa, T. Sumasu, and K. Toko, High photoresponsivity in a GaAs film synthesized on glass using a pseudo-single-crystal Ge seed layer, *Applied Physics Letters* **114**, 142103 (2019).
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Potential of polycrystalline GaAs thin films for wearable solar cells

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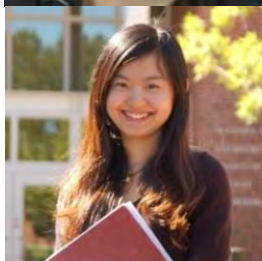
The highest conversion efficiency of solar cells has been updated with III–V compound semiconductors. However, these solar cells use expensive single-crystal Ge or GaAs-based wafers. Therefore, research to synthesize a high-quality GaAs film on an inexpensive substrate has been continuing for decades in the quest to develop a solar cell that achieves both high-efficiency and low-cost. In particular, GaAs solar cells fabricated on flexible plastic substrates will open up the possibility for developing advanced wearable devices. Therefore, we have recently been studying low temperature synthesis of high-quality GaAs films on insulators and achieved the first demonstration of photoresponsivity of the polycrystalline (poly-) GaAs film formed on glass [1,2]. In this study, we controlled the grain size of the poly-GaAs layer over a wide range (1–330 μm) using the Ge seed layers formed on glass by solid-phase epitaxy (SPC) [3–5] and Al-induced layer exchange (ALILE) [6]. With increasing grain size, the photoresponsivity corresponding to GaAs increased from 0.01–3 A W^{-1} under a bias voltage of 0.3 V, indicating the high potential of the large-grained GaAs film. The maximum value approached that of the GaAs film formed simultaneously on a single-crystal Ge wafer and is the highest value ever updated for GaAs films formed at low temperatures on glass. Thus, we experimentally demonstrated the correlation between the grain size of poly-GaAs and its photoresponse property and achieved the pseudo-single-crystal GaAs layer below the heat-proof temperature of general soda-lime glass. Knowledge gained in this study will be essential for designing advanced solar cells based on polycrystalline III–V compound semiconductors using inexpensive substrates. In addition, further lowering the growth temperature ($< 500\text{ }^{\circ}\text{C}$) will lead to novel flexible GaAs solar cells based on plastic substrates. [1] T. Nishida *et al.*, *Applied Physics Letters* **114**, 142103 (2019). [2] T. Nishida *et al.*, *AIP Advances* **10**, 015153 (2020). [3] K. Toko *et al.*, *Scientific Reports* **7**, 16981 (2017). [4] D. Takahara *et al.*, *Applied Physics Letters* **114**, 082105 (2019). [5] M. Saito *et al.*, *Scientific Reports* **9**, 16558 (2019). [6] K. Toko *et al.*, *Journal of Physics D: Applied Physics* **53**, 373002 (2020).



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Martin Janata is at the last year of his undergraduate study with bachelor thesis titled: “coated cerium oxide nanoparticles interaction with cell culture medium”. He is supervised by Dr. Xiaohui Ju, working on the topic of biomedical application of cerium oxide nanoparticles at Charles University, Prague, Czech Republic.

Colloidal stability and catalytic activity of cerium oxide nanoparticles in cell culture media

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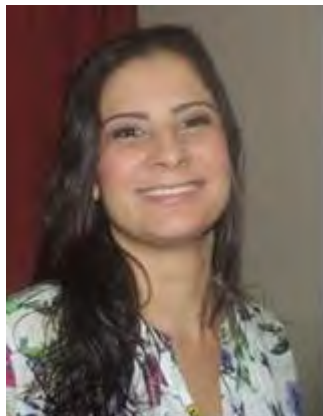
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Martin Janata will be presenting this research.

One of the biggest challenges for the biomedical applications of cerium oxide nanoparticles (CeNPs) is to maintain their colloidal stability and catalytic activity as enzyme mimetics after nanoparticles enter the human cellular environment. This work examines the influences of CeNP surface properties on their colloidal stability and catalytic activity in cell culture media (CCM). Near-spherical CeNPs stabilized via different hydrophilic polymers were prepared through a wet-chemical precipitation method. CeNPs were stabilized via either electrostatic forces, steric forces, or a combination of both, generated by surface functionalization. CeNPs with electrostatic stabilization adsorb more proteins compared to CeNPs with only steric stabilization. The protein coverage further improves CeNPs colloidal stability in CCM. CeNPs with steric polymer stabilizations exhibited better resistance against agglomeration caused by the high ionic strength in CCM. These results suggest a strong correlation between CeNPs intrinsic surface properties and the extrinsic influences of the environment. The most stabilized sample in CCM is poly(acrylic acid) coated CeNPs (PAA-CeNPs), with a combination of both electrostatic and steric forces on the surface. It shows a hydrodynamic diameter of 15 nm while preserving 90% of its antioxidant activity in CCM. PAA-CeNPs are non-toxic to the osteoblastic cell line SAOS-2 and exhibit promising potential as a therapeutic alternative.

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E-mail: anapf.quimica@gmail.com, A.Monteiro@uliege.be<http://www.ceib.uliege.be/>**Optimization of hydroxyapatite texture using CTAB template**

Ana P. F. Monteiro, Gaëlle Idczak, Stéphanie D. Lambert, Christian Grandfils

Interfaculty Research Center of Biomaterials (CEIB), University of Liege, Chemistry Institute, B6c, Allée du Six Août, University Liège, B-4000 Liège (Sart-Tilman), Belgium; Department of Chemical Engineering – Nanomaterials, Catalysis, Electrochemistry (NCE) University of Liège, Allée du Six Août, University Liège, B-4000 Liège (Sart -Tilman), Belgium

Hydroxyapatite (HA), $\text{Ca}_5(\text{PO}_4)_3(\text{OH})$, is a natural ceramic with extensive interest in areas such as biomaterials, adsorbents and catalysis. In the last decades, considerable efforts have been devoted to control the nano-texture of HA, in particular for the sake to increase its total specific surface area and finely tune its porosity at a nanoscale level. To aim that, several approaches have been proposed in the literature, specially using surfactants as molecular template during the synthesis. However, no systematic studies have been published in order to correlate and control the texture properties of HA and the surfactant behavior in the experimental conditions of HA synthesis. This work aims to analyze cetrimonium bromide (CTAB) behavior within conditions simulating HA synthesis in order to better understand and control its aggregation level before considering HA synthesis. To achieve that, CTAB micellisation was evaluated by Dynamic light scattering (DLS) in a concentration ranging from 0.4 to 100 $\text{mmol}\cdot\text{L}^{-1}$ in HA reaction conditions ($\text{pH} = 10.5$ and presence of phosphate ions) at 25 and 50 °C. Interestingly enough at low concentration (i.e. $< 10 \text{ mmol}\cdot\text{L}^{-1}$), CTAB tends to exhibit bimodal population of surfactant aggregates. Above 10 $\text{mmol}\cdot\text{L}^{-1}$ only unimodal size micelles have been distinguished in the autocorrelation curves derived from DLS analysis. No significant difference in CTAB behavior has been noticed at the two temperatures investigated. In a second step several batches of HA have been synthesized adopting CTAB concentration adjusted in function of their aggregation regime. After purification and drying at 100 °C, HA has been analyzed by FTIR, XRD, TGA, BET and TEM techniques. It was clearly observed that the specific surface area of HA can be increased significantly (up to 150 m^2/g) in a narrowed range of CTAB concentration. Moreover, size and shape of HA nanoparticles are remarkably affected by surfactant concentration. From the behavior of CTAB micelles in function of time, temperature and concentrations, the most appropriate medium to perform HA synthesis assisted by CTAB surfactant and its effect in HA texture properties was identified. Additionally, an original feasibility study has highlighted the potency of HA matrix to physisorb, release and keep the stability of Soybean Trypsin Inhibitor (STI), a protein typically adopted as model of Bone Morphogenic Protein (BMP) for tissue engineering purposes

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Picking out iron oxide nanoparticles with custom-made morphology, oxidation state and magnetic response through the selective reagent control

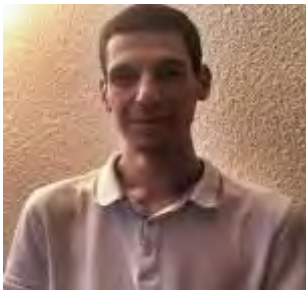
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Iron oxide nanoparticles (NPs) are versatile building blocks in a variety of biomedical and environmental applications due to their good magnetic performance, ease of production and functionalization by chemical routes, and low toxicity. However, controlling the electronic and magnetic properties of iron oxide NPs remain a challenge because of their crucial dependence on composition, structure, surface chemistry, and interparticle interactions. [1, 2]. In this framework, we studied the effect of the amount of both 1,2-hexadecanediol and the solvent 1-octadecene on the thermal decomposition method with iron (III) acetylacetonate. On the one hand, low amounts of either of the two reagents result in large NPs containing both Fe₃O₄ and FeO phases but with high values of the reaction yield. On the other hand, above certain threshold of the reagents the NPs are single-phase, single-crystal Fe₃O₄ NPs with diameters below 10 nm and narrow size distributions, however the reaction yield suffers a slight decrease. Consequently, the samples exhibited two distinct magnetic behaviors depending on the amount of these two reagents. The hysteresis loops at room temperature for the small NPs showed the typical features of superparamagnetism: values of the saturation magnetization close to the bulk one for magnetite with no coercive field. On the contrary, larger NPs showed ferrimagnetic behavior with reduced values of the saturation magnetization, as well as shifted hysteresis loops at 5 K after field cooling the sample at 1 T. The Zero-field cooling-field cooling (ZFC-FC) curves below 200 K for the small NPs showed a peak below room temperature corresponding to the blocking temperature, while those curves for the larger particles displayed two peaks at higher temperatures which can be associated with the Verwey and Neel transitions of magnetite and wüstite phases, respectively. The latter is correlated with the biphasic nature of the large NPs. With this accurate monitoring of the reaction conditions, we have added an extra level of optimization to the synthesis of these NPs. In fact, we have found that, for 1 mmol of iron (III) acetylacetonate, the minimum amounts of 1,2-hexadecanediol and 1-octadecene for the preparation of monophasic, single-crystal Fe₃O₄ NPs are 2.5 mmol and 5 mL, respectively. This allows us to tune the properties of each sample of iron oxide NPs to its specific application. [3] Acknowledgements The work was supported by Spanish MCIU and AEI (MAT2015-68772-P; PGC2018-097789-B-I00) and European Union FEDER funds. M.E-T. acknowledge Spanish MCIU for BES-2016-077527.

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Study grafting density and molecular weight of PMMA-ran-PBMA on Ti by using anew approach with photocleavable initiator

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Titanium (Ti) based plates are generally used to built-up mandibular prosthesis and replace the bone. However, the significant difference of the mechanical properties between Ti and the surrounding tissues results in stress shielding which is detrimental for load bearing tissues. To attenuate this effect, a process with the elaboration of Ti/ PMMA-co-PBMA /Ti sandwich materials (SMS) was developed. We employed surface-confined the poly methyl methacrylate (PMMA)-co- n-butyl methacrylate (PBMA) (PMMA-co-PBMA) layers as adhesives to stick the co-polymer core on the Ti skins to design resin-free SMS by pressing the three components together above the glass transition temperature of the co-polymer. The process route was following: (i) an alkali treatment of Ti surface, (ii) its functionalization with a phosphonic acid-containing polymerization initiator and (iii) controlled radical polymerization of MMA and BMA from this initiator. This work deals with the chemical and physical characterizations of the both copolymers: the core and the grafted on Ti skin. To study the last one, a new photocleavable initiator was designed. The grafting density, molecular weight and also melting point of PMMA-co-PBMA polymer brushes grafted on Ti were determined. Some encouraging results will be discussed.



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**Conductive molecularly imprinted polymer nanotubes
for detection of biomarker proteins at low concentrations**

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Label-free sensor systems are effective methods to detect biomarker proteins for many diseases, however they perform poorly at early detection when concentrations are very low. Integration of nanostructured sensing platforms improves the performance of the sensors by providing larger surfaces to increase sensitivity. Increasing selectivity, as well as the sensitivity, is also needed for the sensors to work efficiently. In this regard, we designed and synthesized conductive molecularly imprinted polymer (MIP) nanotubes to detect biomarker proteins at very low concentrations. Oxidative chemical vapor deposition method was employed to synthesize the nanotubes imprinted with model protein of bovine serum albumin (BSA). As the conductive polymer, PPy (polypyrrole) was chosen due to ease of synthesis. Fourier Transform Infrared (FTIR) analyses validated immobilization and removal of the BSA from the PPy nanotubes and scanning electron microscopy (SEM) results confirmed the formation of the molecularly imprinted PPy nanotubes. UV absorption spectrum was used to detect the adsorption of BSA proteins on the MIP nanotubes at low concentrations. The facile method to synthesize the MIP nanotubes introduced in this study can be applied to other model proteins enabling their integration in different types of sensors.



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Protein Assembly via Thiacalixarene – Metal Complexes

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Protein-based materials are of significance in the search for alternatives to synthetic materials such as plastics. Proteins are highly attractive components for biohybrid materials owing to their biocompatibility and tunable properties. Protein crystals provide order and porosity, which make them interesting for biomaterials. Given the importance of protein materials for biocatalysis, tissue engineering etc., controlled protein assembly is an enabling technology. There are many methods available for protein crystallization, including metal coordination and macrocycle binding (1). The commercially-available, anionic sulfonato-thiacalix [4]arene has potential as a tool in a crystallographer's toolbox for generating protein assemblies. Thiacalixarenes differ from ordinary calixarenes because of their sulfur bridging atoms, allowing for coordination of metal ions and a more flexible macrocycle due to longer carbon-sulfur bonds. Here, we present different protein-thiacalixarene-metal complexes, including the cationic cytochrome *c* and the trimeric lectin from *Ralstonia solanacearum* (RSL). Both zinc and cobalt were studied with these proteins because of their important role in catalysis and protein stability/assembly. The interesting results of our crystal structure analysis will be presented. (1) Guagnini, F., Engilberge, S., Flood, R.J., Ramberg, K.O., Crowley, P.B. Metal-Mediated Protein-Cucurbituril Crystalline Architectures, *Cryst. Growth Des.* 2020, 20, 6983–6989.



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Assessment of surface modification techniques on the corrosion behavior and the ability of apatite formation of titanium

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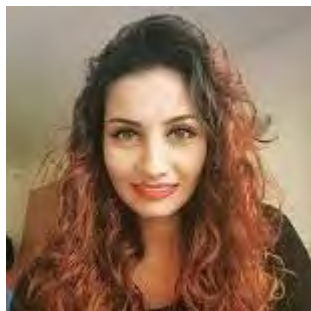
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The use of implants has increased over the years, driven by factors as aging population and desire of patients to maintain the same level of activity and life quality. Furthermore, to tackle the challenges met in the modern medicine, high performance implantable biomaterials must be developed. The most used biomaterial in clinical practice, remain titanium and its alloys, due to their properties and excellent long-term clinical outcomes, being considered “the golden standard”. The paper aim is to assess the impact of different surfaces obtained by metallographic preparation (M), airborne-particle abrasion – (S) and anodization (A) on pure titanium (cp-Ti, grade 2) in terms of bioactivity and corrosion resistance. The M group samples was considered as control and were obtained on SiC papers of different grits (300 ÷1200) and polished with alumina (Al₂O₃) slurry (particle dimensions of 1 μm). The S group were modified by airborne abrasion with alumina particles with dimensions of 250 μm at an air pressure of 3 bars for 20 s. The incidence angle of particle delivery was maintained at 90°. For the A group, the samples were initially etched in a solution HF:HNO₃:H₂O (1:4:5; v/v/v) for 1 min, after which the anodic oxidation was carried out with a DC power supply system by applying a constant voltage of 20 V for 60 min at room temperature in 0.5 wt.% HF solution. The obtained surfaces were characterized in terms of surface morphology, elemental and phasic composition, roughness, wettability, corrosion resistance and in vitro bioactivity by immersion in synthetic body fluid (SBF). The surface modification techniques used in this study have indicated that the bioactive character of cp-Ti can be enhanced through simple and cost-effective methods and can be successfully implemented to obtain medical devices with enhanced features. It was noted that a contact angle lower than 90°, which indicates a hydrophilic surface coupled with a roughness in the nanometric scale (under 200 nm) favor the nucleation and growth of a newly apatite layer, thus indicating an enhanced bioactive character and higher osseointegration. The highest mass of apatite gain in SBF media was found for the surfaces modified by anodic oxidation, while poorer results were noted for the S group. Thus, it was shown that the surface morphology, hydrophilicity, and roughness are playing a crucial role in the biomineralization process. The corrosion tests highlighted that the specimens anodized had also the best performance due to the titanium oxide nanotubes layer which acts as a barrier that inhibits the electrochemical reactions. In conclusion, the present study showed that irrespective of the modification techniques used, the properties of cp-Ti can be tuned.

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Synthesis, hyperthermia tests and anti-melanoma activity of Doxorubicin loaded superparamagnetic iron oxide nanoparticles

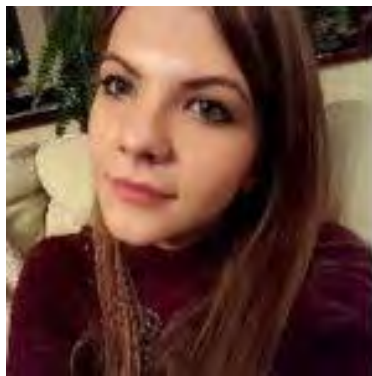
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An alternative method for cancer therapy, which has attracted a significant attention in the past few years, is magnetic hyperthermia. In the presence of RF (radio frequency) magnetic field, the magnetic nanoparticles generate heat, which increase the temperature in tumors in a controlled manner, leading to killing the tumor cells. The interaction between nanoparticles and biological systems depends on the surface modification of magnetic nanoparticles. Cysteine coating enhances colloidal stability, while increasing nanoparticles biocompatibility. Moreover, surface functionalization of magnetic nanoparticles with antitumoral drugs could enable targeted chemotherapeutic delivery during localized hyperthermia. In this study, we report the synthesis of superparamagnetic nanoparticles (SPION NPs) with cysteine, as well as their influence in the hyperthermia study. Biological tests on mouse (B16F10) and human (A375) metastatic melanoma cells confirmed the internalization of magnetic nanoparticles delivering Doxorubicin (Dox), which is used as a chemotherapeutic in the treatment of cancer. The IC50 values of SPION-Cys-Dox were determined for both cell types: 4.26 ug/mL for A375 and 2.74 ug/mL for B16F10 as compared to 60.74 and 98.75 ug/mL, respectively for SPION alone. Treatment of cells with SPION-Cys-Dox has induced decreased pERK activity 3h post-treatment and cell cycle arrest by 48hrs. We have shown that within the first 2hrs of incubation in physiological (pH = 7.4) media ~10-15uM Dox/h is released from a 200ug/mL SPION-Cys-Dox solution, as compared to double upon incubation in citrate (pH = 3), which resembles tumor environment conditions. Based on the obtained results, new perspectives on development of new biocompatible and bio-functional SPION NPs for magnetic hyperthermia are highlighted.

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E-mail: cristina.chircov@upb.ro<https://ro.linkedin.com/in/cristinachircov>**Standardized synthesis of iron oxide nanoparticles through lab-on-chip devices**

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Bogdan Stefan Vasile, Ecaterina Andronescu

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The main goal of the present research work is the development of a standardized method for obtaining uniform nanomaterials. Specifically, we investigated the efficiency of a microfluidic lab-on-chip device for the synthesis of standardized iron oxide nanoparticles with controlled properties in terms of size, shape, crystallinity, and surface charge. The lab-on-chip device was fabricated using a laser machine for the construction of a polymeric plate with screw orifices, three inlets, one outlet, and one cross-junction channel. The device consists of three polymer chips, namely a top chip (with inlets for sample injection and screw orifices for binding), a middle chip (with the cross-junction channel and screw orifices), and a bottom chip (with an outlet and screw orifices), which will be fixed using 20 M4 screws (0.5 mm pitch, 4 mm diameter) and tightened at 1.5–2 Nm. Using two automated syringe pumps, the solutions were simultaneously injected into the lab-on-chip device through Teflon tubes, as follows: the solution containing the Fe(II) and Fe(III) precursors with three different concentrations was injected at three different flows (20, 40, 60 mL/h) into the central inlet, while the solution containing the precipitating agent, NaOH 1M, was injected into the side inlets at 150 mL/h. The nanoparticle dispersions were dripped from the outlet, washed in order to remove secondary reaction products, and dried at 40°C for 48h. The device was characterized through the scanning electron microscopy both before and after the synthesis of the nanoparticles. The synthesized nanoparticles were characterized in terms of morphology, structure, composition, functionality, and stability through electron microscopy (scanning and transmission), selected area electron diffraction, X-ray diffraction, energy-dispersive X-ray spectroscopy, Fourier-Transform infrared spectroscopy, differential thermal analysis and thermogravimetry, and dynamic light scattering. Results showed a deterioration of the device due to its repeated use, demonstrating a limit of 10 experiments that can be performed. Moreover, results proved the presence of iron oxide as the single mineral phase. Additionally, all nanoparticles exhibited uniform spherical shapes and a significantly narrow size distribution below 10 nm. Finally, dynamic light scattering confirmed the dimensional uniformity of the nanoparticles, as the same hydrodynamic diameter was registered for more than 95% of the nanoparticles. Optimal properties in terms of crystallinity, uniformity, and thermal stability were obtained at increasing concentrations and decreasing flows. Therefore, it can be concluded that the lab-on-chip device is an ideal tool for the synthesis of nanomaterials, ensuring the uniformity and standardization necessary for pharmacological applications. As perspectives, it could allow for the one-step fabrication of functionalized nanoparticles and hybrid drug delivery systems with controllable pharmacokinetics.



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The Covalent Immobilization of Heparin to Plasma Polymerized Amine-rich Thin Films on Intravascular Catheter Surfaces

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This paper investigates two different intravascular catheter substrates which were polypropylene (PP) and Titanium (Ti) in here. Both surfaces firstly were exposed to oxygen plasma to increase surface area and produce peroxides on their surfaces. Then substrate surfaces were deposited a thin film of plasma polymeric only ethylene diamine (EDA), besides EDA and NH₃(ammonia) mixtures (1:1, v:v) which is rich in amine groups. Thus, the primary amine groups on the substrate surfaces were used to covalently immobilize heparin. Carboxylic groups of heparin were activated by N-hydroxysuccinimide (NHS) and N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC) or 1,1'-Carbonyldiimidazole (CDI). Eight different plasma modification parameters and two crosslinking agent performances were examined and optimized. The density of immobilized heparin was determined by the Toluidine blue (TB) colorimetric method after immersed in 37°C, DI water with constant shaking for 30

minutes then sonicated for 10 minutes and vortexed for another minute and finally measured at 630 nm wavelength. Heparin stability tests were achieved in phosphate buffer saline (PBS, pH:7.4) medium for a month. The surface-modified PP and Ti substrates were characterized by attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy. The surface topography, hydrophilicity and of the films were investigated by atomic force microscopy and water contact angle measurements.



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Metal Organic Framework UiO-66 Loaded Chitosan Scaffolds for pH-Responsive Drug Delivery

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Osteomyelitis, is the infection of bone with a microbial pathogen-usually *Staphylococcus aureus* and the treatment remains to be a challenge despite the advances in surgical techniques and antimicrobial agents. The difficulties in current clinical approaches are associated with the need for long-term high dose antibiotic therapy and autologous bone grafting to replace the removed necrotic bone tissue. Systems that deliver antibiotics locally have become particularly interesting because of their ability to deliver high concentrations of drugs locally while reducing the systemic toxicity. Moreover, antibiotic loaded implants offer an attractive alternative, as they can not only deliver high-dose antibiotics locally but also replace the dead tissue and promote new bone formation¹⁻³. Metal-organic frameworks (MOFs) composed of metals connected by organic linkers offer many opportunities in biomedical field. Their superior properties like, high porosity, and high drug loading capacity made them attractive in drug delivery applications. Among these structures UiO-66 has recently gained attention due to its non-toxic structure and ease of synthesis. Herein, a potential bone substitute and drug carrier system was prepared to be used in treatment of serious bone infections like osteomyelitis. Fosfomycin, as an antibiotic was loaded into UiO-66 nanocrystals for a pH responsive controlled release. The antibiotic loaded UiO-66 nanocrystals were then incorporated into chitosan scaffolds which were prepared by wet-spinning. Characterization of scaffolds were performed to determine the morphology, swelling behavior and pH controlled fosfomycin release. Antibacterial activity studies were performed to investigate the effectiveness of the scaffolds against *Staphylococcus aureus*. The results showed that fosfomycin loaded into UiO-66 nanocrystals was released in a pH controlled manner from the chitosan scaffolds. Chitosan scaffolds showed a strong effect in the reduction of *Staphylococcus aureus* activity in comparison to chitosan scaffolds alone.

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Synthesis of Metal Organic Framework UiO-66 as an Efficient Antibiotic Vehicle

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Metal organic frameworks (MOF) are a new class of material that has a great potential in drug delivery systems. They possess unique physical and chemical characteristics including large surface area, high drug loading capacity and versatile functionality^{1,2}. UiO-66 is a zirconium-based MOF with very high surface area and unprecedented stability. High chemical, thermal, and mechanical-stability of UiO-66 makes it a perfect candidate for pioneering studies of mechanism and universal applications of general metal-organic frameworks³. Moreover, UiO-66 has recently gained attention as a drug carrier and drug delivery system. In the present work, antibiotic loaded UiO-66 MOF structures have been synthesized for pH controlled delivery. Fosfomycin a small molecule from a unique drug class that acts by inhibiting pyruvyl transferase was loaded to UiO-66 MOF structure both in-situ. The antibiotic loaded UiO-66 nanocrystals were characterized by powder X-ray diffraction, scanning electron microscopy, thermal gravimetric analysis and Fourier-transform infrared spectroscopy. The loading efficiency was determined by liquid chromatography/mass spectrometry analysis. The antimicrobial activity of Fosfomycin loaded UiO-66 nanocrystals were tested against *Staphylococcus aureus* and *Escherechia coli* by using the well diffusion technique. The results demonstrated that a high loading efficiency of ~90% was achieved. The FTIR spectrum for UiO-66 loaded nanocrystals showed the characteristic peaks of pure UiO-66 only, and no bands attributed to fosfomycin indicating the encapsulation of the drug. The crystallinity was reduced but still conserved after encapsulation. The drug loaded UiO-66 nanocrystals showed high antimicrobial activity.

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Magnetite-based nanosystems for improved wound dressings

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The purpose of this study was to obtain and assess the impact of a novel magnetite (Fe₃O₄) nanosystem functionalized with the natural origin compound and antibiotics on the virulence behaviors of some wound pathogens in order to advance research aimed to find alternative and personalized therapeutic approaches for the efficient management of chronic wounds. Magnetite-based nanosystems are efficiently used for the encapsulation and targeted delivery of different biologically active compounds. These nanoparticles have significant potential for the administration of pharmacological substances, as they can enhance biocompatibility, ensure targeted, controlled and prolonged release of therapeutic compounds and reduce the amount of bioactive compound needed for the healing effect desired in many biomedical applications. The crystalline structures of Fe₃O₄ core/shell nanoparticles was identified by X-ray diffraction (XRD) and their dimensions and shapes is observed by high resolution transmission electron microscopy (TEM). Differential Thermal Analysis (DTA) and Thermo Gravimetric analysis (TGA) are coupled in order to determine the stability and thermal degradation of core/shell nanoparticles' components. Our results demonstrated that the use of these nanosystems can ensure optimum intra- and inter-cellular active concentrations, their efficacy being proven in treating different wound infections caused by both Gram-positive and Gram-negative bacteria.

Acknowledgments: This work was supported by a grant of the Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2019-4926, within PNCDI III.

YOUNG INVESTIGATOR FORUM POSTER SESSION
(17.00 h – 18.00 h)

1 KAIQI WU

17.00 (O.YIF.P1) ABSTRACT CONTROL ID number UBVX6

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Dr.

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**QUANTUM SENSING TO INVESTIGATE INTRACELLULAR FREE
RADICAL RESPONSE UPON BACTERIAL INFECTIONS BY USING
NANODIAMOND-BACTERIAL CONJUGATE**

Kaiqi Wu

Romana Schirhagl, University of Groningen, NL

Low concentrations of reactive oxygen species (ROS) mediate various signaling processes in phagocytic cells (e.g. macrophages) when infected by bacteria [1]. Production of a suitable probe is needed to measure these events. However, most methods used to investigate the intracellular ROS share the same problems, including photobleaching, low sensitivity, lack of spatial and temporal resolution [2]. Here, we elucidate the utility of diamond magnetometry for studying the transient free radical response of macrophages upon *Staphylococcus aureus* (*S. aureus*) infection, without influence on the intracellular redox reactions or enzymatic activity. Nitrogen-Vacancy (NV) defect centers in diamond crystals can detect magnetic noise nearby (< 10 nm), which is produced by the spin of unpaired electrons of free radicals³. Diamond magnetometry is specific for paramagnetic ROS also called free radicals (for example nitric oxide, superoxide anion radicals, or hydroxyl radical) [4]. They are particularly important since they are the most reactive ROS[1,5,6]. In this study, we report the formation and characterization of nanodiamond-bacteria conjugates, *S. aureus*-FNDs. By using these conjugates, we can optically monitor the transient free radicals in phagosomes via measuring the spin-lattice relaxation (T₁) of NV defects after macrophages internalized the conjugates. In conjunction with appropriate control groups, bacteria-FNDs conjugates appear to be a powerful tool for unraveling bacteria-infected pathways and pathogenesis that involve free radicals. References [1] Dupré Crochet, S.; Erard, M.; Nü'e, O., ROS production in phagocytes: why, when, and where? *Journal of leukocyte biology* 2013, 94 (4), 657-670. [2] Nüsse, O., Biochemistry of the phagosome: the challenge to study a transient organelle. *TheScientificWorldJOURNAL* 2011, 11. [3] Perona Marti'nez, F.; Nusantara, A. C.; Chipaux, M.; Padamati, S. K.; Schirhagl, R., Nanodiamond Relaxometry-Based Detection of Free-Radical Species When Produced in Chemical Reactions in Biologically Relevant Conditions. *ACS Sensors* 2020. [4] Morita, A.; Nusantara, A. C.; Martinez, F. P. P.; Hamoh, T.; Damle, V. G.; van der Laan, K. J.; Sigaeva, A.; Vedelaar, T.; Chang, M.; Chipaux, M., Quantum monitoring the metabolism of individual yeast mutant strain cells when aged, stressed or treated with antioxidant. *arXiv preprint arXiv:2007.16130* 2020. [5] McCord, J. M.; Fridovich, I., The utility of superoxide dismutase in studying free radical reactions I. radicals generated by the interaction of sulfite, dimethyl sulfoxide, and oxygen. *Journal of Biological Chemistry* 1969, 244 (22), 6056-6063. [6] Wang, Q.; Ding, F.; Zhu, N.; Li, H.; He, P.; Fang, Y., Determination of hydroxyl radical by capillary zone electrophoresis with amperometric detection. *Journal of Chromatography A* 2003, 1016 (1), 123-128.

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Hydrophilic Polyvinylidene fluoride coatings obtained via MAPLE deposition and their in vitro preliminary osteoblast response

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New advances in biomedicine field have concentrated on producing novel and stable surfaces that can stimulate a specific cellular response toward the demands of implants and medical devices. Among these materials, polyvinylidene fluoride (PVDF) are considered of high interest for biomedical research area due to its a number of characteristics that make it a versatile biomaterial, insolubility, stability in biological media, in vitro and in vivo non-toxicity, or even piezoelectric properties. Nonetheless, the most important disadvantage of PVDF-based biointerfaces is associated to the absence of the functional groups on the fluoropolymer and its hydrophobic character conducting to a deficiency of cell adhesion and proliferation. Within this context, this work aims to investigate the obtaining of PVDF coatings by matrix assisted pulsed laser evaporation (MAPLE) and the in vitro response of MC3T3-E1 pre-osteoblast cells towards the surface microarchitecture. MAPLE deposition parameters and post-deposition thermal treatment were studied for optimizing and designing the morphological features of the coatings, while maintaining the chemical characteristics similar to those of the pristine material. In vitro studies with MC3T3-E1 pre-osteoblasts indicated good biocompatibility, with no significant alteration of the cell adhesion and viability after the thermal treatment of the coatings. The physico-chemical characteristics of the deposited coatings along with favorable in vitro osteoblast response demonstrate that MAPLE is an adequate method for obtaining PVDF coatings for future bio- applications.



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Dr. Monica Marini is a Senior Postdoc at the Department of Applied Science and Technology (DISAT) of the Polytechnic of Turin in Italy. Her research focuses on the mechanical and structural study of nucleic acids and their interactions with other biomolecules (e.g., Rad51 repair protein) and ligands such as chemotherapeutic compounds (Cisplatin), bis-intercalants (YOYO-1) and heavy metals (e.g. Nickel) to reveal their connection to diagnosis and disease. To reach this goal, conventional bio -molecular, -chemical and -physical tools are combined with microfabrication, high-resolution TEM imaging and diffraction, Raman spectroscopy, and Laser Doppler Vibrometer.

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Suspended DNA self-sieving and characterization over superhydrophobic surfaces: a Raman spectroscopy study

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Oriented and self-organized DNA filaments were obtained by micro-fabricated super-hydrophobic surfaces (SHS). The bio-macromolecule, suspended over the SHS, can be characterized by using several techniques, such as electron microscopy and optical spectroscopy. DNA direct imaging by high resolution TEM (HRTEM) allowed solving the base pairs with a resolution of 1.5 Å [1,2] and the metrological details can be effectively corroborated by Raman spectroscopy data [3,4]. Raman spectra in the range 600-1800 cm⁻¹ were acquired on suspended DNA filaments and on the droplet residual. The spectra obtained at the same working conditions on DNA samples and buffer deposited over a CaF₂ window were used as negative control. The study of the spectra revealed the absence of physiologically compatible buffers on suspended filaments while their contribution is strong in the DNA spectra acquired on CaF₂ windows and on the droplet residual. This suggests that the optimized SHS platform separates small molecules from the suspended DNA and the non-interacted material is concentrated in the droplet residual. The SHS-DNA platform revealed a strong potential for the study of polarized Raman spectra as the DNA filaments are autonomously oriented with different angles over the device and for the analysis of the presence and influence of molecules affecting the DNA double helix such as chemotherapeutic compound (Cisplatin), heavy metals and methylations.



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Ph.D student. Alexina Ollier

Alexina Ollier is Ph.D student of University of Basel supervised by Prof. Ernst Meyer. She has started her PhD program on January 2019 as a part of the Swiss Nanoscience Institute that is a center of excellence for nanosciences and nanotechnology. Her research interests are energy dissipation on 2D materials and quantum systems using the pendulum geometry atomic force microscope. The technique enables to measure energy loss of free-standing graphene sheets.

Prof. Ernst Meyer

Ernst Meyer is Professor of Physics at University of Basel, Switzerland. He obtained his Ph.D at the University of Basel in 1986. His research interests include SPM methods (AFM and STM) at different conditions (UHV, low temperature, high temperature, magnetic field ...) and molecular systems such as spray deposition and studies using different sensors. For the remarkable achievements regarding these studies, he has won several awards and has published over 300 peer-reviewed papers with approximately 20'000 citations in total.

Referred Journals Publication List

1. A. Ollier, M. Kisiel, R. Pawlak, U. Gysin, E. Tosatti and E. Meyer, Energy dissipation on suspended graphene, in preparation.
2. A. Ollier, M. Kisiel, U. Gysin and E. Meyer, Low frequency noise in suspended graphene, in preparation

PhD student Alexina Ollier –**Invited Presenter at The Young Scientist Forum The E-MRS Symposium “Bioinspired and bio integrated materials as new frontiers nanomaterials” Xth Edition (The E-MRS Spring Meeting 2020 Strasbourg).**

Low frequency noise in suspended graphene

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Understanding nanoscale energy dissipation is nowadays among few priorities particularly in solid state systems. Breakdown of topological protection, loss of quantum information and disorder-assisted hot electrons scattering in graphene are just few examples of systems, where the presence of energy

dissipation has a great impact on the studied object. It is therefore critical to know, how and where the energy leaks. High sensitivity pendulum geometry Atomic Force Microscope (pAFM), oscillating like a pendulum over the surface, is perfectly suited to measure tiny amount of dissipation. The tip position on the sample is controlled with atomic accuracy owing to a tunnelling current line and the enhanced sensitivity allows to distinguish between electronic, phononic or van der Waals types of dissipation.

In this work we performed energy dissipation measurements on a suspended graphene sheet at room temperature under UHV. The graphene is deposited on a hole patterned substrate to have suspended circular (diameter of 6.5 μm) graphene sheet. The experiments allow to investigate the phononic and electronic energy dissipation of the suspended graphene. In addition to that, random charging and discharging events are also observed on the free-standing membranes.

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Filip Grajkowski is an undergraduate student at Trinity College Dublin, Ireland conducting research under the supervision of Prof. Paula E. Colavita. His research interests include the functionalisation of carbon-based electrodes for applications in analytical and bioanalytical chemistry. His recent work has involved the fabrication of carbon electrode materials with specific active moieties to discern the influence thereof on the electroanalytical performance and stability of these materials for the sensing of species such as dopamine. This is facilitated by a fabrication approach that combines sputtering deposition and post-deposition thermal and electrochemical treatments, along with a combined characterisation approach involving electrochemistry, x-ray photoelectron spectroscopy and atomic force microscopy. He is also knowledgeable in the area of catechol chemistry, with an understanding of the physicochemical properties of these compounds and their behaviour in electroanalysis. He has previously been awarded a scholarship to pursue this work from the Laidlaw Foundation as part of the Undergraduate Research and Leadership Programme. Lastly, he is the co-author of a peer-reviewed publication, with a further two in preparation.

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- (1) Behan, J. A.; [Grajkowski, F.](#); Jayasundara, D. R.; Vilella-Arribas, L.; García-Melchor, M.; Colavita, P. E., Influence of carbon nanostructure and oxygen moieties on dopamine adsorption and charge transfer kinetics at glassy carbon surfaces. *Electrochimica Acta* 2019, 304, 221-230.

Challenges in Dopamine Sensing at Carbon Electrodes: Dopamine Adsorption Properties and Electrode Fouling at Physiological pHFilip Grajkowski¹, James A. Behan¹, Alessandro Iannaci¹, Paula E. Colavita¹¹*School of Chemistry, CRANN and AMBER Research Centres, Trinity College Dublin, College Green, Dublin 2, Ireland*

Due to its role in the operation of nervous response and renal, hormonal and cardiovascular systems, quantitation of dopamine (DA) *in vivo* has received great interest. Electrochemical sensing allows detection of nanomolar dopamine concentrations, and carbon-based electrodes are particularly suitable for this application due to their biocompatibility, ease of manufacture, low cost and functionalisation potential. However, carbon electrode current responses are influenced by DA-surface interactions and suffer from fouling by adsorption and accumulation of oxidation by-products, collectively called ‘polydopamine’ (PDA). Herein, we present a study of DA adsorption at carbon electrodes functionalised with N-/O-groups and the fouling properties thereof at physiological pH. Electrodes with smooth, reproducible morphologies, tuneable functionality types and concentrations and, crucially, tuneable sp³/sp² ratios were synthesised via sputtering deposition and thermal/electrochemical treatments. The influence of surface graphitisation and surface chemistry was investigated using cyclic voltammetry and x-ray photoelectron spectroscopy to rationalise the connection between DA adsorption and electrode fouling, with preliminary AFM studies characterising the surface roughness. The ability of fouled surfaces to recover their sensing ability was also evaluated using acid cleaning and repeated fouling, to elucidate factors which promote/inhibit PDA adsorption. Our results suggest effective methods for optimising carbon electrode composition as a means of minimising fouling in DA electroanalysis.

This work has partly emanated from research conducted with the financial support of Science Foundation Ireland under Grant No. 13/CDA/2213. JAB acknowledges support from the Irish Research Council under Grant No. GOIPG/2014/399. FG acknowledges the support of the Laidlaw Undergraduate Research and Leadership Programme.



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

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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 (Pr. 19-72-20180).



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Dr. Silambarasan Anbumani is a Post-doctoral research fellow at the Institute of Physics 'Gleb Wataghin' (IFGW) of the University of Campinas, Brazil since June 2018. His current research interest includes tailoring surface properties, and development of functional nanomaterials, polymers, and micro/nanostructured scaffolds for biomedical applications. His research also includes the nucleation kinetics and crystallization to produce high quality single crystals for laser applications. He was the recipient of the São Paulo Research Foundation (FAPESP) Post-doctoral fellowship, Government of Brazil - in 2018, National Post-doctoral Fellowship in 2017, and Young researcher International travel grant in 2016 from Science and Engineering Research Board(SERB), Government of India. He has published 16 peer-reviewed research publications and 20+ conference presentations/invited talks and received 2 externally funded R&D projects as a principal/co-investigator.

Tailoring surface physicochemical SU-8 properties to modulate bacterial mobility, adhesion and biofilm formation

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SU-8 is an epoxy-based photoresist which has been used as a novel platform for biomedical applications due to its chemically tunable and biocompatible surface in addition to its relatively high stiffness, chemical resistance, optical transparency and ease of processing properties. In this work, we tailor SU-8 surface properties to investigate single cell motility and adhesion of the bacteria *Xylella fastidiosa*. Different SU-8 samples have been prepared using UV illumination, thermal processing, and oxygen plasma treatment. Atomic Force Microscopy and X-Ray Photoelectron Spectroscopy were used to determine nanoscale surface properties; ex-vivo studies at the level from single cell to biofilm formation were carried out with Confocal Laser Scanning Microscopy (CLSM). The mean velocity and displacement of single cells have been extracted from CLSM tracking information data and the size and quantity of biofilms are compared for different samples. We observed a significant difference in bacterial cell motility, adhesion and also biofilm architecture on SU-8 as nanoscale surface property changes. Larger density of carboxyl groups in SU-8 surfaces provide enhanced cell motility, while denser biofilms are found in untreated SU-8. Our results can improve understanding of the role of nanoscale properties on bacteria-surface interaction and thereby create strategies to preventing microbial adhesion and consequently, biofilm development of pathogenic species.



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Dr.Eng. Alina Vladescu, has a B.S. in Materials Science and Engineering from the University Politehnica of Bucharest (2002) and an MS in Biomaterials from the Department of Bioengineering and Biotechnology, University Politehnica of Bucharest (2004). Her PhD however is in Materials Science from University Politehnica of Bucharest (2011). She works at National Institute for Optoelectronics, Department for Advanced Surface Processing and Analysis by Vacuum Technologies. She is also associate professor in Surface Engineering at University Politehnica of Bucharest. She is also affiliated as research scientist at National Research Tomsk Polytechnic University.

Expertise: • Functional coatings (metals, nitrides, carbides, oxides and oxynitrides) deposited by magnetron sputtering and cathodic arc techniques), especially for optics, optoelectronics, mechanical and tribological applications, but also with special properties, such as corrosion resistant and biomaterials. • Oxide thin films by electron gun evaporation technique, especially for optoelectronics applications and (again) for biomaterials. • Analysis and characterization of thin films using various spectroscopies (UV-Vis-NIR, EDS), X-ray diffraction, morphological, mechanical, anticorrosion and tribological characterization.

Guest Editor: *Frontiers in Materials* (2016-2017), *Composite Interfaces* (2016), *Coatings* (2019-2021).

Consequently, she has 123 technical publications and presentations, 10 patents, 3 books. Most of these articles have involved the surface biofunctionalization of metallic components of the biomedical devices by PVD deposition methods. In general, these articles have primarily proved that both PVD techniques (reactive magnetron sputtering and vacuum cathodic arc) represent a valuable choice for coating the metallic femoral heads, determining the increase of their service-life. Up to date she was involved in the investigation and assessment of various types of coatings, such as: nitrides, carbides, carbonitrides, oxynitrides or oxides, in mono and multilayered structures.

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Preparation of CaP doped Mg coatings used for biomedical applications

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In biomedical applications, it is new challenge to reducing the implant failure risk due to bacterial infection and/or poor osteointegration. The best solution is to develop new implants' generation with highly customized and made of resorbable materials. The aim of the current poster is to investigate the CaP doped Mg coatings as possible resorbable material used for biomedical applications. The coatings were prepared by RF magnetron sputtering method on silicon wafers substrates. Comparatively investigations were carried out in terms of their elemental and phase composition, mechanical characteristics (roughness, hardness, adhesion, elastic modulus), and degradation rate in SBF and DMEM at 37°C. CaP coating without Mg addition was used as reference coating. We acknowledge the support of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project ERANET-M-ISIDE-1, no. 171/2020 (INOE2000 partner) or 112/2020 (UPB partner), within PNCDI III, and no. 19PFE/2018 (PROINSTITUTIO) – institutional project.



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Anita Ioana Visan career highlights involves: materials science; surface engineering by UV excimer lasers and laser-material interactions; Thin films(Laser-Assisted Processing by Pulsed Laser Deposition (PLD), Matrix Assisted Pulsed Laser Evaporation (MAPLE), CAD/CAM Rapid Prototyping by Matrix Assisted Pulsed Laser Evaporation Direct Write (MAPLE DW) & Reverse MAPLE - a novel chemical templating approach for controlled-release drug delivery systems). She have studied different biomaterials: pure/doped biomimetic hydroxyapatite; biopolymers (Polyethylene glycol (PEG); Polycaprolactone (PCL); chitosan; Poly(3-hydroxybutyric-acid-co-3-hydroxyvaleric-acid) (PHVB); poly(lactic-co-glycolic acid) (PLGA); polyaniline grafted lignin); Proteins: (Lysozyme, Silk Fibroin (SF)); Bacteria: (E. coli, S. aureus, B. subtilis, E. faecalis strains); Antimicrobial: (flavonoids; poly(1,3-bis-(p-carboxyphenoxy propane)-co-(sebacic anhydride)) /gentamicin sulfate; quercetin, resveratrol, lignin). She applied in her studies techniques for Material and Surface Investigation(e.g. FT-IR Spectrophotometry; Atomic Force Microscopy: AFM; Electron Microscopy: SEM, HRTEM; Electron Spectroscopy: XPS, AES). In special she focused on Biomedical Applications: Drug Delivery, Tissue Engineering, Faster Diagnosis and Treatment, Biofouling, Bio-chem sensors, Antimicrobial assays and 3D Printing. The originality of her results is confirmed by the publication of 19 ISI Indexed articles (5 – first author; 14 – co-author) in scientific journals of Q1, 1 book chapter; summing a Total citations of 265, Hirsh index: 10 - according to Scopus; Total citations: 250 (221 without self-citations): Hirsh = 9; according to Web of Science; Total citations: 315, Hirsh = 10 according to Google Scholar. (ResearcherID: I-7288-2016; ORCID 0000-0003-0539-4160). She is the project leader of a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2020-2273, within PNCDI III. She also has got favorable recognition by winning the national fellowship program L'Oréal—UNESCO “For Women in Science”. Her international visibility is demonstrated by the involvement as a member of local organizing committee of 10th International Conference on Photoexcited Processes and Applications, as well as more than 75 participations at scientific communications (including 23 oral presentations and invited lectures) at National and International conferences, workshops and seminars in the related field. One note that during her research activity she won 1 Best Poster Awards and 2 Best Oral Presentations.

Biodegradable Polymeric coating matrices for drug-eluting stents

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Polymer-coated stents with antiproliferative drugs and growth factor have been proposed to defeat adverse reactions which occur in cardiovascular treatment. We report on successful deposition of functionalized thin films of (everolimus and paclitaxel) drugs encapsulated in complex matrices [either blends of poly(L-

lactide) and collagen or nanoparticles of poly(lactic-co-glycolic acid) - polyvinyl alcohol] containing vascular endothelial growth factor (VEGF) by Matrix Assisted Pulsed Laser Evaporation (MAPLE). The morphology, hydrophilicity, and biodegradability of the composite coatings have been investigated. The main recipes of the drug functionalized polymer matrices, synthesized by MAPLE, have been validated by biological investigations, drug release profiles, and physical-chemical investigations. In vitro evaluation tests performed on the fabricated thin films have revealed great biocompatibility, that may endorse them as competitive candidates for the development of improved non-toxic surfaces resistant to microbial colonization. The proposed functionalized thin films apart from preventing the restenosis (due to selected drug inhibitors), also could eliminate the risk of late thrombosis (as the covered stent is replaced by connective tissue thanks to VEGF addition) and are expected to act as improved/appropriate/effective coatings for the next-generation drug-eluting stents.

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Mariona Escoda-Torroella is a predoctoral student in the Magnetic Nanomaterials Group at the University of Barcelona. She was trained as a Chemist and studied the Master in Nanoscience and Nanotechnology. In 2016 she started her Ph.D. at the Magnetic Nanomaterials Group (UB) at the Faculty of Physics. And currently her research is focused on the synthesis by chemical routes and the characterization of nanoparticles. She is working to make hybrid nanomaterials using nanoparticles of different materials to obtain combinations of plasmonic and magnetic properties, as well as a good response as X-ray contrast agents.

Controlling the morphology and composition of Bi₂S₃ nanoneedles decorated with gold nanospheres

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Computed tomography (CT) is an X-ray based whole body imaging technique widely used to enhance the contrast among human body tissues because it allows both enhanced tissue penetration and resolution imaging. Currently, clinically approved CT contrast agents are iodinated molecules or barium suspensions, but to provide a good image contrast, high doses are required, and their short circulation time limits their applications. Nanoparticles (NPs) show several advantages in comparison with small molecules, such as longer blood residence times, and a high potential for cell-tracking and targeted imaging applications due to their easy surface functionalization. Bi₂S₃ NPs are interesting as they present a large X-ray attenuation coefficient because of the Bi atoms, which strongly enhances the image contrast for small variations in the concentration of NPs present in the target tissue. Moreover, Bi is less expensive and exhibits lower toxicity than other metals with a similar X-ray attenuation coefficient. In addition, the combination of Bi₂S₃ with Au offers the possibility of adding extra functionalities to these nanostructures. In particular, Au NPs exhibit strong absorption associated with localized surface plasmon resonances and show biocompatibility, stability, and low toxicity, making them suitable for photothermal therapies. In this work, Bi₂S₃ NPs with different size and shape have been prepared by tuning the temperature and the reaction time in the hot-injection synthesis of a sulfur precursor. On the one hand, when the injection is performed at 105 °C with short reaction times, spheroid-shaped particles are obtained that grow preferentially along the direction [001] as the reaction time increases, giving rise eventually to needle-shaped particles. On the other hand, injecting at 165 °C, rod-shaped NPs are obtained regardless of the reaction time. Once the structural features of the Bi₂S₃ NPs were controlled, we added an additional step to the synthesis process to achieve hybrid materials with both Bi₂S₃ nanoneedles and Au nanospheres attached on the surface. With this combination, we expect to prepare a novel, multifunctional, hybrid material with potential for theranostics. Acknowledgements The work was supported by Spanish MCIU and AEI (MAT2015-68772-P; PGC2018-097789-B-I00) and European Union FEDER funds. M.E-T. acknowledges Spanish MCIU for PhD grant BES-2016-077527.

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BIOINSPIRED HYDROXYAPATITE TREATED WITH COLD PLASMA FOR DENTAL APPLICATIONS

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Despite the technological progress of the last decade, dental caries is still the most frequent oral health threat in children and adults alike. Such condition has multiple triggers and is caused mainly by enamel degradation under acidic attack of microbial cells, which compose the biofilm of the dental plaque. The aim of this study was to elaborate a cold plasma based method in order to modulate microbial attachment and biofilm formation and to improve the retention of fluoride in an enamel-like model composed of bioinspired hydroxyapatite (HAP). HAP model was obtained by hydrothermal method using synthWAVE Microwave Synthesis System and characterized by FTIR spectroscopy, SEM, TEM and SAED. HAP fluoridation was done by applying an optimized Plasma gun treatment under atmospheric pressure. Antimicrobial analysis was done by qualitative and quantitative methods using Gram positive (*Staphylococcus aureus*) and Gram negative (*Pseudomonas aeruginosa*) model strains. The obtained results revealed the obtained HAP particles have nanometric sizes and needle type crystalline morphology, ranging 10-20 nm. Purity and basic properties of the obtained HAP correspond to ICSD-203027 (Cod.Ref.: 01-080-7087). Plasma gun treatment revealed that Fluoride content is increased in the HAP treated samples, after the application of fluoridated gel, as compared to plasma untreated samples. Microbial viability assay demonstrated that the obtained plasma treated HAP bear significant antimicrobial properties, since both *S.aureus* and *P aeruginosa* viability is drastically decreased after less than 4 h of exposure. The obtained cold plasma treated HAP structure could be efficiently used in dental applications and prevention of dental caries, by inhibiting the development of microbial pathogens.

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Nanochip for personalized assessment of checkpoint immunotherapy

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Immune checkpoint blockade has been extensively explored as a novel and promising antitumor treatment, these checkpoints help keep immune responses from being too strong and sometimes can keep T cells from killing cancer cells. When these checkpoints are blocked, T cells can kill cancer cells more efficiently. Yet this is largely challenged by low frequency of response, and the risk of developing autoimmune side effects. Whether and how the regulation of T-cells by the clustering of activating and inhibitory receptors is tumor dependent, and patient dependent is still to be investigated. Furthermore, does this regulation correlates with the patient sensitivity to PD-1 blockade by a commonly used PD-1 blocker Pembrolizumab (KEYTRUDA)? If it does, can it be exploited to predict patient responsiveness to the checkpoint blockade? To address these questions, we developed nanochip devices for the precise assessment of anti-tumor immunotherapy. These devices were designed with various nanoclusters of activating and inhibitory ligands which engage the receptors of T-cells. These nanochips were used as an artificial tumor cell, and help test T-cells from different patients on different nanochip arrays, with and without the PD-1 blocker drug Pembrolizumab, in order to study how the T-cells response to different patterns of the ligand clusters correlates with patient sensitivity to PD-1 blockade. This research has provided an important insight into the fundamental mechanisms of immune checkpoint blockade, and pave the way to the development of a novel nanochip technology for the personalization of this promising antitumor immunotherapy.

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Effect of inorganic nanoparticles on probiotic and microbiota isolated bacteria strains

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From ingested food, to the use of daily products that can be easily ingested, and also to the use of nanosized drug delivery systems for therapy, resident microbiota is exposed to nanoparticles (NPs) in widely undiscovered ways. The aim of this study is to investigate the in vitro interactions among inorganic NPs widely encountered in common practices and cultivable microbiota and probiotic isolates. Four types of inorganic NPs which are widely encountered in daily use products, namely CuO, Ag, Fe₃O₄ and ZnO were synthesized in this study. CuO and ZnO NPs were obtained by hydrothermal method, Ag by chemical reduction and Fe₃O₄ by co-precipitation. All NPs were physico-chemically characterized by SEM, TEM and FTIR spectroscopy. Microbiological analysis was performed by using four microbiota isolated strains with probiotic potential (2 strains of *Enterofoccus faecalis* and 2 strains of *Lactobacillus rhamnosus*), which were identified from newborn stool by MALDI-TOF. Our results demonstrated that the obtained NPs have round shape and variable size, ranging between 10-100 nm, depending on their type. Lowest size was obtained for the Fe₃O₄ NPs (10-15 nm). *E.faecalis* and *L.rhamnosus* strains were exposed to the obtained NPs for various type periods and the results demonstrated that Ag NPs are the only to exhibit a significant antimicrobial effect in the tested conditions. The other tested NPs showed however some effects in the attachment and other phenotypes which are important for the anti-pathogenic effects of microbiota and probiotic strains. The obtained data supports the idea that inorganic NPs could interfere with some biological processes in microbiota strains with probiotic potential, and this could impact on the development of some metabolic diseases.



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Madalina Handrea-Dragan is a physicist PhD student at Babes-Bolyai University from Cluj-Napoca, Romania, being supervised by Dr. Ioan Botiz. Her doctoral research work is focused on the development of micro and nanostructured polymeric materials as base platforms which can be interfaced with nanoparticles of various functionality. With these structures she expects to develop unique optical and electronic properties which can be further used both in technological and biological applications. She is also actively involved in two research projects at Nanobiophotonics and Laser Microspectroscopy Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, UBB Cluj in which she is working on subjects related to the development of optoelectronic devices and also to the fabrication of nanoparticle-based biosensing platforms.

Gold nanoparticle micro-stripes as sensing platforms for human B lymphocyte-specific antigen detection

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Gold nanoparticles (GNPs) and their assemblies have been widely used as building blocks for the fabrication of (bio)sensing devices, grace to their unique optical and electronic properties, large surface to volume ratio and easy surface modification. The effectiveness of such nanostructures as transducing elements in optical sensors based on surface plasmon resonance (SPR), surface-enhanced fluorescence (SEF) or surface-enhanced Raman spectroscopy (SERS) was repeatedly demonstrated and many efforts have been devoted to tailor and control the morphology, solubility, surface functionality and stability of GNPs' constituent elements. In this work we propose an optical biosensor assay capable of exploiting both SPR and SERS-based detection of the recombinant human B-lymphocyte antigen CD20, a protein involved in the regulation of B-cell activation and proliferation. The device consists of micro-stripes that were formed via oriented self-assembly deposition of closely packed spherical GNPs within pre-patterned polymeric grooves. The stripes formation was characterized by optical and scanning electron microscopy. The effect of particle size and shape, lateral periodicity of grooves and antigen concentration on the detection sensitivity in various matrices, was thoroughly investigated. By using a Raman reporter in the detection scheme, herein Fluorescein isothiocyanate (FITC) pre-conjugated onto anti-CD20 antibodies, the proposed device is able to function for the multimodal detection and identification of the targeted analyte. Such nanoparticle-based sensing platforms fabricated by a nontoxic and simple route are promising for applications in biochemistry and the medical field. Acknowledgement: This work was supported by the project PN-III-P1-1.1-TE-2016-0919.



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Enrico Bianchetti is a PhD student at the University of Milano-Bicocca, supervised by Prof. Cristiana Di Valentin, head of the NanoQlab research group. He is a computational chemist within the fields of materials science and nanotechnology. His research focuses on transition metal oxides nanosized systems for biomedical applications, such as magnetic resonance imaging, targeted drug delivery and hyperthermia therapy. In particular, he studies Fe_3O_4 surfaces and nanoparticles in vacuum and in presence of water and organic molecules to investigate structural, electronic, and magnetic properties of such promising nanomaterials. Furthermore, he is currently collaborating with Prof. Suresh Pillai (Institute of Technology Sligo, Ireland) on a project related to doped- TiO_2 for catalytic and energetic applications. His DFT-based simulations are carried on through out CRYSTAL17 and DFTB+ codes.

Parametrization of the $\text{Fe-O}_{\text{water}}$ cross-interaction for a more accurate $\text{Fe}_3\text{O}_4/\text{water}$ interface model

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Iron oxides/water interfaces are involved in many fundamental and technological processes (*Q. A. Pankhurst, J. Connolly, S. K. Jones, and J. Dobson, J. Phys. D: Appl. Phys. 36, R167 (2003); A. K. Gupta and M. Gupta, Biomaterials 26, 3995 (2005)*), therefore accurate force field parameters for the description of the bond between surface iron sites and water oxygens are critical to perform useful molecular dynamics simulations in this fast-developing research field. In a previous work by my group (*H. Liu, E. Bianchetti, P. Siani, and C. Di Valentin, J. Chem. Phys. 152, 124711 (2020)*), the behaviour of water multilayers with increasing thickness up to 12 nm on the low-index (001) Fe_3O_4 facet has been investigated comparing density functional tight binding (DFTB+U) results with molecular mechanics molecular dynamics simulations. However, the classical model that we used, although catching the general aspects of the water structure and of solvation, has shown limited accuracy in the description of the details of the water coordination to the exposed surface undercoordinated iron sites. In the abovementioned model, longer distances ($\sim 2.7\text{-}2.8\text{\AA}$) between the superficial iron atoms and the oxygen atoms of adsorbed water molecules ($\text{Fe-O}_{\text{water}}$) have been observed compared to higher-level calculations using hybrid density functional theory (HSE06) and DFTB+U methods that predict $\text{Fe-O}_{\text{water}}$ distances about 2.2 Å. In the new work by my group (*P. Siani, E. Bianchetti, H. Liu, and C. Di Valentin, J. Chem. Phys. 154, 034702 (2021)*), a set of CLASS2 force field parameters is optimized to properly describe the $\text{Fe-O}_{\text{water}}$ cross interaction through comparison with hybrid DFT (HSE06) calculations of the potential energy function for a single water molecule adsorbed on the Fe_3O_4 (001) surface and with DFTB+U molecular dynamics simulations for a water tri-layer on the same surface. The performance of the new parameters is assessed through the analysis of the number density profile of a water bulk (12 nm) sandwiched between two magnetite slabs of large surface area. Their transferability is tested for the water adsorption on the curved surface of a spherical Fe_3O_4 nanoparticle of realistic size (2.5 nm).



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Dr. Lia-Mara Ditu is Associate Professor at University of Bucharest, Faculty of Biology. Experience and expertise: Project leader in national research projects; member in 11 national research projects whose research directions include: evaluation of microbicidal / microbiostatic / anti-pathogenic (QS inhibitors) effects of newly synthesized chemicals, probiotics and herbal extracts and optimization of the methodology for selecting and characterizing their biological activities; study of the interaction of nanoparticles and nanostructured hybrid systems with planktonic and adherent microbial cells. She teaches courses and practical works of Epidemiology, Industrial and Medical Microbiology, for bachelor and master students, approaching the aspects related to the composition of human microbiota, microbial pathogen virulence, Nosocomial Infections

Novel photocatalytic activated resin formula for microbial colonization control

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The development of antimicrobial coatings with increased efficiency for the protection of critical surfaces is an important goal in finding new systems for medical area surfaces. The aim of the present study was to develop a novel photocatalytic activated product based on resins, in order to prevent and control the microbial pathogens implicated in healthcare associated infections. To achieve the purpose, the research team designed different formulations based on acrylic / acrystyrene-styrene resins in aqueous dispersion and formulations based on acrylic resin dilutable with OH approx. 2.5%, with additional anatase grade TiO₂ pigment doped with metal oxides. All samples were chemical (UV-VIS, IR spectra) and physical characterized, including the optimal lifetime test (by exposure to different chemical and physical external-environmental factors). The antimicrobial activity was evaluated using qualitative and quantitative methods (according with adapted CLSI 2020 standard method), after incubation in different conditions of light radiation, including darkness. The microbial strains used for the experiments were represented by both clinical and standard microbial strains (*Staphylococcus aureus* ATCC 25923, *Enterococcus faecalis* ATCC 29212, *Pseudomonas aeruginosa* ATCC 27853, *Escherichia coli* ATCC 25922, *Candida albicans* ATCC 10231). Our results demonstrated that the obtained photocatalytic activated resins formula showed very good viscosity, hardness and drying time, with stability over time. Also, the antimicrobial tests showed significant inhibitory effect, with the decrease of CFU/ml values by at least 4 log., especially when the incubation was performed by exposure to radiation with the spectral range between 450 nm and 500 nm. This results demonstrated that the tested formula induced toxic biological effects after photocatalytic activation, considering them as light-activated antimicrobial agents-LAAAs and offering long time antimicrobial and mechanical protection of surfaces with high risk of contamination, in order to prevent and combat the spread of pathogenic microorganisms.

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Dr. Grumezescu is an impressive young post-doc researcher, who is always in search for novel studies and approaches in her work. Although her main research activity is based on the engineering and chemistry of nanostructured materials, her skills have also improved significantly during the last years in the fields of biology, and laser processing. These interconnected acquired skills have therefore allowed her to develop cutting-edge research in the field of bioactive nanomaterials and laser-processed surfaces.

Her valuable research is supported both by an impressive number of publications (+70 research papers and 13 book chapters focused on novel and multifunctional nanostructured materials with applications in various medical fields), and a *H*-index of 20.

Bioactive coatings based on hydroxyapatite for biofilm modulation

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Nanostructured coatings for surface modification of metallic implants are of great interest for orthopedic and orthodontic applications, especially given their potential to boost an implant's osseointegration and to provide local antimicrobial activity. The aim of this study was to modify metallic surfaces with nanostructured bioactive coatings based on hydroxyapatite (HAp) nanoparticles and biomolecules, so as to improve biological activity and limit the formation and development of Gram-positive and Gram-negative bacterial biofilms. The obtained composite materials based on HAp were proposed as multifunctional coatings for hard tissue implants. The functionalized nanoparticles were characterized by TEM, SAED, SEM, EDS, XRD and FT-IR. Composite coatings were fabricated by Matrix Assisted Pulsed Laser Evaporation (MAPLE) technique, following thorough fluence studies to identify optimum conditions for laser processing. Complementary IRM and SEM investigations were performed in this respect. The biological activity of nanostructured samples was quantitatively and qualitatively assessed on eukaryotic cells, which evidenced the highly biocompatible behavior of proposed materials. Microbiological results have demonstrated that the bioactive HAp-based coatings significantly inhibited the contamination and colonization of different microbial species. The laser processed nanostructured coatings developed in this study could represent an efficient approach in developing bioactive platforms with anti-infective ability to be used in implantology. Acknowledgments: Contract PN-III-P1-1.1-PD-2019-1185, project number: PD 142/2020

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Dr. Grumezescu is an impressive young post-doc researcher, who is always in search for novel studies and approaches in her work. Although her main research activity is based on the engineering and chemistry of nanostructured materials, her skills have also improved significantly during the last years in the fields of biology, and laser processing. These interconnected acquired skills have therefore allowed her to develop cutting-edge research in the field of bioactive nanomaterials and laser-processed surfaces.

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Fe₃O₄ nanoarchitectures functionalized with eugenol for modulation of virulence and biofilm formation

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The purpose of this study was to obtain and evaluate a novel magnetite nanosystem functionalized with natural-derived eugenol (Fe₃O₄@E), as well as to assess its impact on the most frequently isolated pathogens from skin infections, including strains responsible for G-tube-related complications. Physicochemical results demonstrated that the average size of obtained nanosystem was 10-20 nm, particles were relatively homogenous and had a reduced tendency to form aggregates. Subinhibitory concentrations of Fe₃O₄@E limited biofilm formation in a time- and strain-dependent manner, and significantly inhibited the production of toxin pore forming enzymes. Inflammatory cytokine release was assessed in human diploid cell cultures grown in the presence of Fe₃O₄@ core-shell nanosystem and as-modified G-tube surfaces. Besides excellent anti-adherence and antibiofilm effects, the proposed nanomaterials proved high biocompatibility, allowing the normal development and growth of human endothelial cells. This approach could be successfully applied for the optimization of medical devices' surfaces in order to control and prevent microbial contamination and colonization and biofilm-associated infections. Acknowledgments: Contract PN-III-P2-2.1-PED-2019-3829, project number: PED 505/2020