Welcome

The Centro de Física das Universidades do Minho e do Porto (CF-UM-UP) was founded in 2014 but the history of its parts, the Centro de Física da Universidade do Minho (CFUM) and the Centro de Física do Porto (CFP), began in the 20-th century. With more than 100 members, more than 80 holding a PhD, CF-UM-UP is the largest academic Research Centre in Physics located in the North of Portugal. CFUM is strongly involved in interdisciplinary research and development activities and the team includes Physicists, Materials Scientists, Mathematicians, and specialists in Optics (including that of human eye) and Optometry. CFP is fully devoted to research in theoretical physics, in the broad area of Quantum Physics and Fields in High Energy and Condensed Matter. The very idea of creation of the CF-UM-UP was to explore the complementarity of the two Centres and achieve synergies in research across disciplines, with a robust backbone of fundamental Physics.

Does it work? This workshop, the Jornadas CF-UM-UP 2019, where all members of the Centre, of all its research lines were invited to participate, is expected to give at least a partial answer to this question. As a clearly positive sign.
I notice the impressive number of nearly 140 registered participants, with 2 keynotes, 4 invited and 5 contributed talks and over 70 posters to be presented. Such a high interest to the Jornadas is partially owing to the announced contests for the Best Oral and Poster Presentation Awards (an excellent idea of the organizers!), but certainly it is also because of the opportunity to attend the keynotes and invited talks and see what other researchers around are doing. This book of abstracts gives a clear idea of the broadness of research topics at the CF-UM-UP and I believe that many of them will be interesting to the majority of the Centre's members when presented during the workshop.

I welcome you to the Jornadas and express my very special thanks to the organizers, Ana Rita Rodrigues, Bruno Amorim and Joel Borges.

Mikhail Vasilevskiy

CF-UM-UP Director

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Scientific Committee

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RoundTable "The importance of research in the innovation challenges and needs of industry"

Filipe Vaz (Moderator)

Senentxu Lanceros-Méndez

Lorena Diéguez, CEO RubyNanomed & INL Staff Researcher

Eliseu Vieira, Bosch Head of Engineering Department in Braga

Alexandre Marques, ZF Group I&D Centre Administrator in Portugal

Cláudia Azevedo, ANI Interface Unit Coordinator

Programme

8h30 – 9h00	Registration
	Opening Session
9h00 – 9h10	Mikhail Vasilevskiy, Director of CF-UM-UP
	Morning Session
	Contributed Talks — Chair: Senentxu Lanceros-Mendez
9h10 – 9h25	**TopoSEM: a simple software tool to obtain three-dimensional surfaces from images of Scanning Electron Microscopy** Diego Martinez-Martinez
9h25 – 9h40	**Magneto-optical Kerr effect in spin split two-dimensional massive Dirac materials** Gonçalo Catarina
9h40 – 9h55	**Microfluidics for controlled self-assembly of cubosome nanoparticles of tunable size** Celso Ferreira
9h55 – 10h10	**Stationary Quantum Transport in Finite Fermionic Systems** João P. Santos Pires
10h10 – 10h25	**Development of a High-Resolution Localized Surface Plasmon Resonance Bio- and Gas-Sensing System using Nano-Designed Thin Films of Au-TiO_2** Marco S. Rodrigues
10h25 – 11h20	Poster Session, Vote for Best Oral Presentation & Coffee Break
	Keynote Speaker — Chair: Filipe Vaz
11h20 – 12h00	**New strategies towards high performance and low temperature processing of solution process metal oxide TFTs** Elvira Fortunato, CENIMAT/i3N Departamento de Ciência dos Materiais, FCT, Universidade NOVA de Lisboa & CEMOP/UNINOVA
	Invited Talks — Chair: Pedro Alpuim
12h00 – 12h20	**Transparent Thermoelectric TiO_2:Nb Thin Films** Carlos Tavares, CF-UM-UP, Universidade do Minho
12h20 – 12h40	**Exploring the Spectral and Temporal Dependence of Nonlinear Optical Effects in Graphene** César Bernardo, CF-UM-UP, Universidade do Minho
12h40 – 14h00	Lunch Break

Afternoon Session		
	Keynote Speaker	Chair: José Manuel Meijome
14h00 – 14h40	**Light, Vision and Eyes: History and Modern Optics** Luis Miguel Bernardo, Departamento de Física e Astronomia da Universidade do Porto	
	Invited Talks	Chair: José Manuel Meijome
14h40 – 15h00	**Magnetoelectric biomaterials for cell response modulation** Margarida M. Fernandes, CF-UM-UP & CEB, Universidade do Minho	
15h00 – 15h20	**Measuring valley polarization with second harmonic generation, and other nonlinear optics experiments with 2D crystals** José Carlos Viana Gomes, CF-UM-UP, CA2DM & Graphene Research Centre, National University of Singapore	
15h20 – 15h30	Poster Session	
15h30 – 16h05	Flash Poster Presentations	Chair: Ana Rita Rodrigues
16H05 – 16h30	Poster Session, Vote for Best Flash Poster Presentation & Coffee Break	
	Round Table Discussion	Moderator: Filipe Vaz
16h30 – 17h45	**The importance of research in the innovation challenges and needs of industry** Filipe Vaz, Prorector of Research and Projects at UM & CF-UM-UP Researcher Senentxu Lanceros-Méndez, CF-UM-UP Researcher Lorena Diéguez, CEO RubyNanomed & INL Staff Researcher Eliseu Vieira, Bosch Head of Engineering Department in Braga Alexandre Marques, ZF Group I&D Centre Administrator in Portugal Cláudia Azevedo, ANI Interface Unit Coordinator	

Closing Session	
17h45 – 18h00	Best Presentation Awards & Concluding Remarks

Keynote Speakers

New strategies towards high performance and low temperature processing of solution process metal oxide TFTs

Elvira Fortunato

*CENIMAT/i3N Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia (FCT), Universidade NOVA de Lis boa (UNL), and CEMOP/UNINOVA, 2829-516 Caparica, Portugal *e-mail: emf@fct.unl.pt*

Abstract: Solution-based metal oxides have been attracting a lot of attention due to the low cost, high throughput a nd simple chemical composition control when compared with vacuum-based systems. These materials have outst anding properties such as high optical transparency, chemical and thermal stability and mechanical toughness. A lso, facile tailoring of solution-based metal oxides leads to multifunctionality allowing their application in different a reas, like sensing, energy and flexible displays. Particularly for large-area electronics the exploration of a crucial co mponent, the thin film transistor (TFT) and their key materials components, the semiconductor, the dielectric, the conductor as well as substrate are demanded. To boost the implementation of TFTs emerging printing techniques and low thermal budget, novel approaches have been and need to be further explored. This paper focuses on rec ent low temperature approaches as combustion synthesis, ultraviolet post annealing treatments which allow their implementation in printable flexible TFTs.

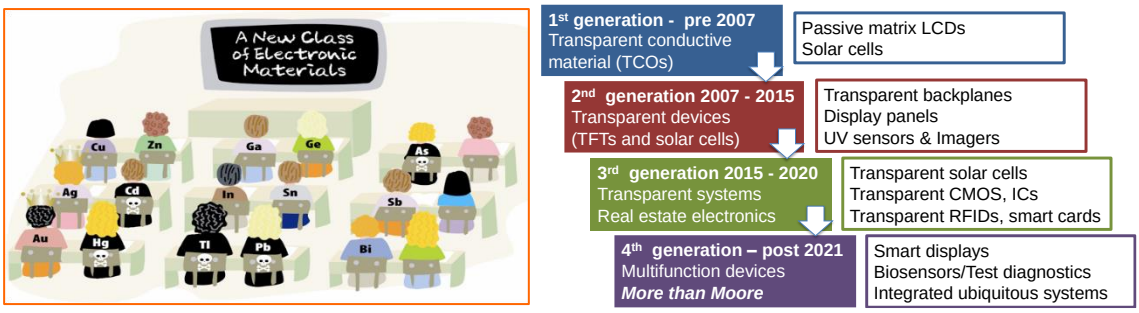

Figure 1. A comparison between a classroom and the new class of electronic materials based on metal oxides, by Prof. J. Wager from Oregon State University and the evolution of metal oxide materials..

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Acknowledgments: This work is funded by ERC AdG project DIGISMART ref. 787410.

Light, Vision and Eyes: History and Modern Optics

Luis Miguel Bernardo

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Keywords: Light, Colour, 3D Vision, Eyes

Abstract: Surrounded by electromagnetic solar energy, marine and terrestrial living beings have evolved using that energy to extend their lives and ensure the survival of their species. They used a well-defined luminous spectral band and, in order to gain information about their surroundings, also used light phenomena, acquired visual capacities appropriate to their needs and developed image-forming and detecting organs compatible with their ways of life. The organs of vision developed by the animals followed many and varied evolutionary pathways and the refractive eyes stood out among the various solutions, providing many species of animals including humans. The human eye presents a good resolution, discriminates colors and, through binocular stereoscopy, provides three-dimensional vision (3D). The refractive defects that often arise in the human eye limit vision and have significantly conditioned the lives of many of our ancestors. Efforts have been made since the thirteenth century to correct these defects, either throughout the use of spectacles or contact lenses or through some surgical procedures that modify the shape of the cornea or implant intraocular lenses. In this presentation the above subjects will be discussed under historical and scientific perspectives highlighting some examples of visual abilities, based on complex and unusual processes, and some creative ways to correct the refractive defects of the eyes.

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Invited Talks

Transparent Thermoelectric TiO_2:Nb Thin Films

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Keywords: Thermoelectric, metal oxide, thin films, X-ray absorption near edge structure, sputtering

Abstract: The design of a transparent conducting oxide (TCO) material with thermoelectric properties is a promising technology for touch–screen displays and solar cell applications. In this work, Nb-doped TiO_2 thin films were deposited by d.c. magnetron sputtering. By modifying the optical, electric, thermal and thermoelectric properties of the produced TiO_2:Nb thin films, enables their suitability for thermal energy harvesters in devices in order to render these more sustainable. For optimized deposition conditions, ~100 nm thick TiO_2:Nb thin films with an optical transmittance up to 85 %, a relatively low electrical resistivity (>10^{-2} Ω·cm), low thermal conductivity (<2 $W \cdot m^{-1} \cdot K^{-1}$), and a high absolute Seebeck coefficient (>200 $\mu V \cdot K^{-1}$) corresponding to a power factor of 125 $\mu W \cdot K^{-2} \cdot m^{-1}$ and ZT figure of merit close to 0.1, were attained. Both anatase and rutile crystalline phases were identified in the X-ray diffractograms. Detailed information on the local structure of the thin films was obtained from radial distribution functions determined from simultaneous analysis of X-ray absorption data at two absorption edges using reverse Monte Carlo method. X-ray photoelectron spectroscopy experiments confirms that Nb^{5+} ions substitute Ti^{4+} in the TiO_2 lattice, providing a charge unbalance to the matrix. Furthermore, due to larger ionic radii, Nb^{5+} scatter phonons more efficiently and reduce the thermal conductivity, which is essential for enhancing the thermoelectric property.

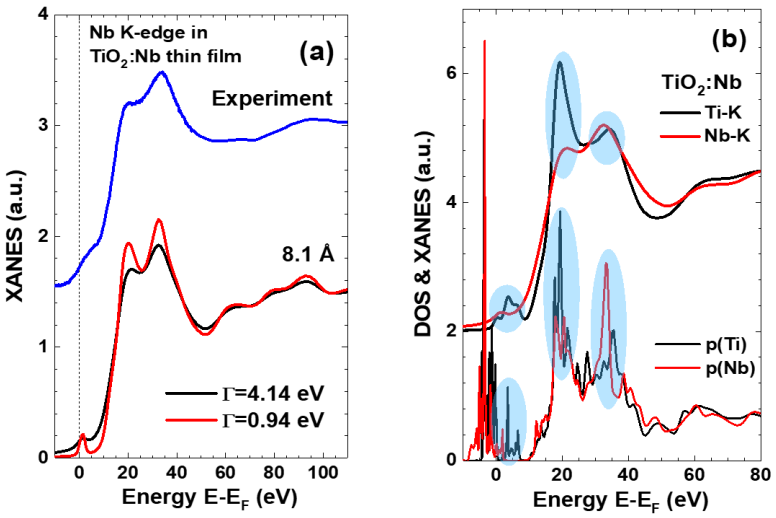

Figure 1. (a) Experimental and calculated Nb K-edge XANES spectra of TiO_2:Nb thin film. The calculations were performed for the cluster radius of 8.1 Å and two different core-level widths Γ=0.94 eV and 4.14 eV. (b) A comparison of the calculated XANES spectra at the Ti and Nb K-edges (top) with p-DOS for Ti and Nb (bottom).

Acknowledgements: Filipe Correia is grateful to the Fundação para a Ciência e Tecnologia (FCT, Portugal) for the Ph.D. Grant SFRH/BD/111720/2015. Joana Ribeiro is grateful to the Project WinPSC - POCI-01-0247-FEDER-017796, for the research grant, co-funded by the European Regional Development Fund (ERDF), through the Operational Programme for Competitiveness and Internationalisation (COMPETE 2020), under the PORTUGAL 2020 Partnership Agreement. We acknowledge the funding from Fundação para a Ciência e Tecnologia (FCT, Portugal) / PIDDAC through the Strategic Funds project reference UID/FIS/04650/2013.

Exploring the Spectral and Temporal Dependence of Nonlinear Optical Effects in Graphene

Cesar Bernardo*[1], Diogo Cunha[1], Manuel Rodrigues[1],Fátima Cerqueira[1,2], Pedro Alpuim[1,2], Michael S. Belsley[1], Mikhail I. Vasilevskiy[1].

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Keywords: Graphene, Nonlinear, Kerr effect, hybrid structures.

Abstract: Graphene is an atomically thin two-dimensional material with remarkable optical properties. Graphene presents a nearly uniform and surprising high absorption across the visible and near infrared as well as a strong third order nonlinear optical response. (Bonaccorso et al., 2010) Under strong laser illumination, graphene exhibits both a transmittance increase due to saturable absorption and a nonlinear phase shift induced via the Kerr effect making the graphene a promising candidate for optical signal processing applications in integrated photonics. However, researchers have measured a wide range of values for the nonlinear refractive index using different characterization methods. To date no clear picture of the optical nonlinearity has emerged.

By means of the cross phase modulation via the ultrafast optical Kerr effect method, we characterize the third-order nonlinear response of graphene and compare it to experimental values obtained by four wave mixing(Hendry et al., 2010), OHD-OKE (Optical Heterodyne Detection of the Optical Kerr Effect) (Dremetsika et al., 2016), and Z-scan methods (Miao et al., 2015; Thakur et al., 2019). From these measurements we identify both real and imaginary parts of the complex nonlinear refractive index our CVD monolayer graphene. We find that graphene the nonlinear changes induced by a strong pump ultrashort field can temporally alter the refractive index seen by a weaker probe field and observe a strong dependence on frequency. This effect hold promise for developing a high-speed all-optical switch based on graphene.

Furthermore, we explored how combining Graphene with Quantums dots (QDs) or Nanosheets (NSs) to create artificial nanostructures might reinforce their respective strengths. These materials can be coupled via exciton-plasmon or exciton-exciton interactions. We have probed this coupling using Raman spectroscopy, Time-Correlated Single Photon Counting (TCSPC), Ultrafast Transient Absorption Spectroscopy (TAS) and Time-Resolved Second Harmonic Generation (TR2HG) in an attempt to characterize the underlying physical processes and evaluate the potential technological significance of these hybrids structures.

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Acknowledgements: SFRH/BD/102616/2014 & POCI-01-0145-FEDER-029265 PTDC/NAN-OPT/29265/2017

Magnetoelectric biomaterials for cell response modulation

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Keywords: magnetoelectric, electrically active biomaterials, cells, bacteria, cells modulation

Abstract: The ability of cells to adapt to different physicochemical environments and external signals is gaining increased scientific attention from advanced materials perspective and modulation of cellular response. Therefore, the application of physical stimuli are being continuously explored to modulate cell functions in a controlled manner. For instance, the use of magnetic cues on magneto-electrical/mechanical scaffolds are being explored as a promising strategy also for remote stimulation of bone and its regeneration in a process called mechanotransduction [1], in which cells are able to sense the forces and translate them into desired biochemical and biological responses. Similarly, bacteria is also sensitive to these type of stimuli, and a controlled shear mechanical stress has been shown to beneficially affect bacterial cell adhesion and proliferation [2], improving their capacity to infect the host. This work reports on the development of novel magnetolectric biomaterials intended to be used for advanced applications in biomedicine. These materials are nanocomposites processed in different forms such as films, 3D scaffolds, electrospun fibres and membranes. As a piezoelectric component, polyvinylidene fluorine (PVDF) and its co-polymers or silk fibroin was used, while $CoFe_2O_4$ NPs or Ni nanowires (Nws) were developed as a magnetostrictive component. These magnetoelectric scaffolds react to the magnetic field provided by the magnetic bioreactor by providing an electrical polarization variation in the piezoelectric phase of the composite. Changing the conditions by which the stimuli are given, as well as the structure of the magnetoelectric material, the behaviour of mammalian and bacterial cells may be tailored. The proper conditions have been outlined for stimulation of bone tissue regeneration, as well as for the development of antimicrobial or promicrobial surfaces, a very important feature to obtain novel strategies for fighting antimicrobial resistance.

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Measuring valley polarization with second harmonic generation, and other nonlinear optics experiments with 2d crystals

José Carlos Viana Gomes

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CA2DM & Graphene Research Centre, National University of Singapore

Keywords: 2D semiconductors; valley polarization; harmonic generation; Transition metal dichalcogenides

Abstract: Two-dimensional (2D) crystalline semiconductors and their heterostructures exhibit a range of remarkable optical properties that offers immense potential to photonic and quantum information technologies. After the groundbreaking work done in graphene, other 2D materials such as Transition Metal Dichalcogenides (TMDs), Balck Phosphorous (BP) or hexagonal Boron Nitride (hBN), were extensively studied and, in particular, in their optical properties. Most (if not all) of these exciting properties are related to the photophysical properties of excitons, bound states of electrons and holes, which in these materials are particularly robust due to a very large binding energy. They are the responsible for the strong nonlinear response of TMDs and BP and, when isolated as a quantum state, for the single-photon emission in TMDs and hBN. In addition to the charge and spin degrees of freedom (exploited in electronics spintronics), excitons in TMDs have the ability to induce, sustain, and control a valley polarization which endows yet another way to encode and process information (coined as valleytronics). In this talk, I will present some of the work done in my group, in close collaboration with other groups at NUS, one at the Center for Advanced 2D Materials (CA2DM) and another at the Center Quantum Technologies in Singapore, in the study of optical properties of 2D crystals and their integration in photonic platforms and waveguides. In particular, I will present some results on harmonic generation and detection of valley polarization in TMDs, the fabrication of polymer waveguides used to encapsulate and optically address 2D crystals, and on recent efforts in single-photon generation in hBN and exciton trapping in TMDs. I will finish commenting on possible future collaborations between the CA2DM and the CF-UM-UP.

Contributed Talks

Magneto-optical Kerr effect in spin split two-dimensional massive Dirac materials

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[2] *Centro de Física das Universidades do Minho e do Porto and Departamento de Física and QuantaLab, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal*
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Keywords: Magneto-optical Kerr effect, 2D massive Dirac electrons, spin-orbit coupling, exchange spin splitting, diluted magnetic impurities

Abstract: Two-dimensional (2D) massive Dirac electrons possess a finite Berry curvature, with Chern number $\pm 1/2$, that entails both a quantized dc Hall response and a subgap full-quarter Kerr rotation. The observation of these effects in 2D massive Dirac materials such as gapped graphene, hexagonal boron nitride or transition metal dichalcogenides (TMDs) is obscured by the fact that Dirac cones come in pairs with opposite sign Berry curvatures, leading to a vanishing Chern number. Here, we show that the presence of spin-orbit interactions, combined with an exchange spin splitting induced either by diluted magnetic impurities or by proximity to a ferromagnetic insulator, offsets this cancellation, leading to an anomalous Hall response that results in a net magneto-optical Kerr effect in such systems. We focus on the case of TMD monolayers at charge neutrality and study the dependence of Kerr rotation on frequency and exchange spin splitting. The role of the substrate is included in the theory and found to critically affect the results. Our calculations indicate that state-of-the-art magneto-optical Kerr spectroscopy can detect a single magnetic impurity in diluted magnetic TMDs.

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Acknowledgements: G. C. acknowledges Fundação para a Ciência e a Tecnologia (FCT) for Grant No. SFRH/BD/138806/2018. G. C. and J. F.-R. acknowledge financial support from FCT through Grant No. P2020-PTDC/FIS-NAN/4662/2014. N. M. R. P. acknowledges financial support from European Commission through project "Graphene-Driven Revolutions in ICT and Beyond" (Ref. No. 785219), FCT in the framework of Strategic Financing (Ref. No. UID/FIS/04650/2019), and COMPETE2020, PORTUGAL2020, FEDER and FCT for Grants No. PTDC/FIS-NAN/3668/2013, No. POCI-01-0145-FEDER-028114, No. POCI-01-0145-FEDER-029265 and No. PTDC/NAN-OPT/29265/2017. J. F.-R. acknowledges FCT for Grant No. UTAP-EXPL/NTec/0046/2017, as well as Generalitat Valenciana funding Prometeo2017/139 and MINECO-Spain (Grant No. MAT2016-78625-C2).

Microfluidics for controlled self-assembly of cubosome nanoparticles of tunable size

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Keywords: Cubosomes, Solvent Shifting, Microfluidics, Controllable Size

Abstract: Cubosomes are nano-sized dispersions of bicontinuous cubic phases, ideal to deliver bioactive molecules in therapeutic applications[1]. They are typically prepared either by fragmenting the cubic phase in excess water using high energy input, or using solvent-shifting approaches[2]. In both cases, poor experimental control at the micron-scale (e.g. poor control on concentration gradients), limits the fine tuning of the particle properties and results in cubosomes with broad size distributions. In this work, we employ the solvent-exchange method using a COC microfluidic device[3], achieving rapid and controlled mixing at the micron-scale and obtaining Monoolein:F127 cubosomes of tunable size and low polydispersity. The micron-sized channels in microfluidics lead to laminar flow regimes and enhanced experimental control. In this regime, hydrodynamic focusing can be used to decrease the mixing time between different components, by decreasing the distances that molecules must travel for total mixing. An ethanol-lipid solution is flowed in a central inlet, which is squeezed by two side streams of water with stabilizer. As the lipid-ethanol solution narrows, ethanol and water are mixed in a controlled way by diffusion, leading to formation of cubosomes (figure). By manipulating the flow rate ratio (Q_R) between the two solutions we manipulate the width in which the hydrodynamic focusing occurs, influencing the assembly time in a homogeneous way. Hence, by manipulating Q_R, we can tune the sizes of cubosomes. Nanoparticle size is a key parameter in drug delivery. Being able to control it is therefore a relevant step towards the design of new and more efficient formulations.

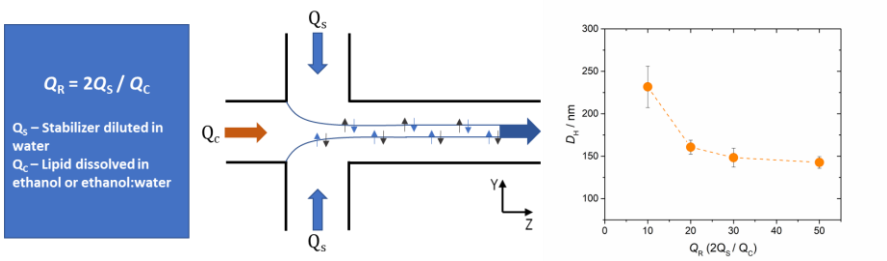

Figure 1: *Schematic representation of the experiment setup. The calculated Q_R is used to manipulate the ratio in which the side solutions (Q_S) and centre solution (Q_C) are injected inside the microfluidic device. As the Q_R is changed inside the device, the centre solution has its width decreased which results in a shorter mixing time between the solvents. The change in time is translated in different particle sizes. The obtained samples from the device are later characterized using Dynamic Light Scattering (DLS).*

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Acknowledgements: This research is supported by Microfluidic Layer-by-layer Assembly of Cationic Liposome - Nucleic Acid Nanoparticles for Gene Delivery project (032520) co-funded by FCT and the ERDF through COMPETE2020.

Development of a High-Resolution Localized Surface Plasmon Resonance Bio- and Gas-Sensing System using Nano-Designed Thin Films of Au-TiO_2

Marco S. Rodrigues*, Rui M.S. Pereira, Mikhail I. Vasilevskiy, Joel Borges, Filipe Vaz

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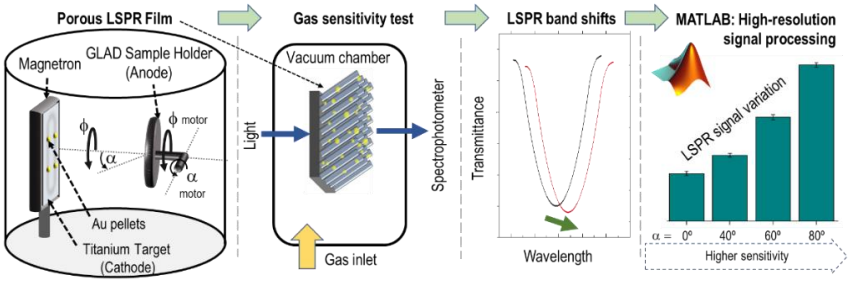
Keywords: LSPR, Gold nanoparticles, Magnetron sputtering, Optical sensing, Signal processing.

Abstract: Localized Surface Plasmon Resonance (LSPR) phenomenon is a hot topic due to the unique optical properties of metal nanoparticles and nanostructures. The optical response of these materials can be tailored [1] by changing the size, shape and distribution of the nanoparticles, as well as the surrounding dielectric matrix. GLancing Angle Deposition (GLAD) is a powerful thin film preparation technique that allows attaining unusual architectures such as inclined columns, zigzags, spirals, among others. When optimizing those architectured and porous thin film systems, with embedded Au nanoparticles, analyte molecules can diffuse easily to their vicinity and thus the thin films can reveal unique sensing responses to various types of environments, namely biomolecules and noxious gases. These interactions can be detected through optical techniques [2,3] by monitoring the characteristics of the LSPR band, in transmittance mode (T-LSPR). This work combines (i) the preparation of nanostructured plasmonic thin films, using GLAD angles up to 80°; (ii) LSPR extinction band processing using an algorithm; and iii) high-resolution LSPR gas sensitivity tests. The signals obtained from the refractive index sensitivity studies were processed using an algorithm that analyses changes in several parameters of the LSPR band, including the central moments of the normalized spectral distribution. The results showed that the developed high-resolution LSPR spectroscopy system, combined with the software algorithm, is a powerful tool for a real-time analysis of the sensor's response. Furthermore, the tailoring of the film's morphology and nanostructure was achieved by GLAD, whereby higher incidence angles manifested enhanced sensitivities.



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Acknowledgements: This research was funded by FCT in the framework of the Strategic Funding UID/FIS/04650/2019; and by the project NANOSENSING POCI-01-0145-FEDER-016902, with FCT reference PTDC/FIS-NAN/1154/2014. Marco S. Rodrigues acknowledges FCT for his PhD Scholarship, SFRH/BD/118684/2016.

TopoSEM: a simple software tool to obtain three-dimensional surfaces from images of Scanning Electron Microscopy

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Keywords: SEM, Digital Image Correlation, 3D, reconstruction topography

Abstract: In this work we describe a new patented method called TopoSEM that allows reconstructing the topography of a surface using a set of at least 3 SEM images acquired at different tilting angles [1, 2]. In that regard, the output is similar to what is obtained by conventional AFM measurements (Figure 1). This method is based on Digital Image Correlation of the images and a posterior analysis of the displacement field according to a rigid-body model. The advantages of this approach are threefold. First, the method does not require any detailed knowledge of the geometry of the chamber or the movement of the stage, and therefore no complex calibration processes are needed. Second, the method is fully software-based and it can be implemented in any SEM equipment. Third, this approach works at any magnification used by SEM, which can be an advantage over AFM devices.

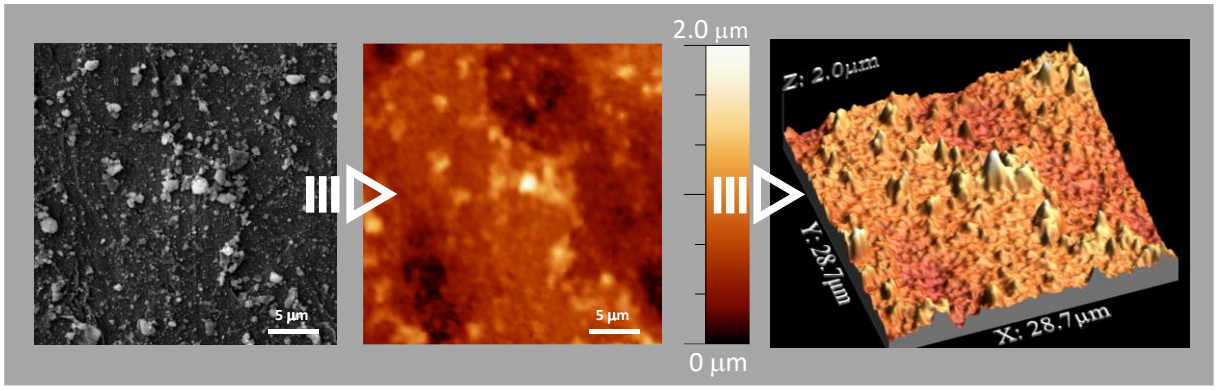

Figure 1 – Example of the results of TopoSEM software. Left: original SEM image. Center, right: two representations of the 3D surface reconstruction. [2,3]

First, the main steps of the approach will be described, including a brief explanation of the mathematical background. Next, its applicability and accuracy will be illustrated with examples from materials science and biology, where the first operative version of the software will be presented as well. Finally, an outlook summarizing future directions of developments and improvements to solve some detected issues will be discussed.

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Stationary Quantum Transport in Finite Fermionic Systems

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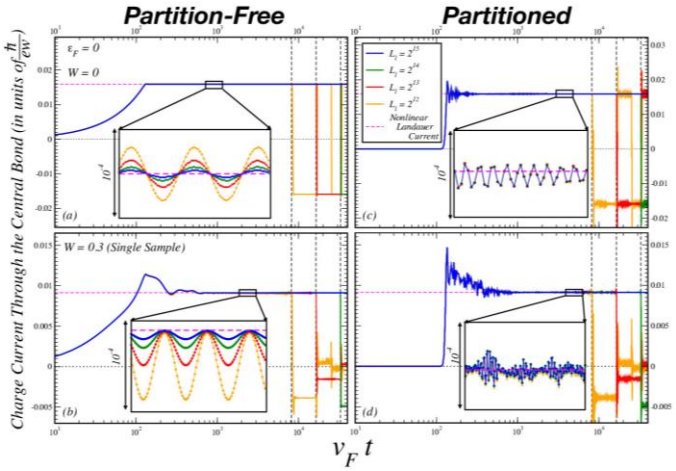
Keywords:1D Fermionic Systems, Mesoscopic Transport, Quantum Dynamics, Landauer Formula, Finite-Lead Effects



Abstract: I will present comprehensive numerical study of an emergent Landauer transport regime from the quantum-mechanical dynamics of free electrons in a disordered tight-binding chain, which is coupled to finite leads with open boundaries [5]. We observe that for large enough leads and for intermediate times, a spatially uniform quasi-steady-state transport emerges, which coincides with the Landauer current [1], and is independent of the initial state of the system, agreeing with Ref. [2]. We fully characterise the local current's time-dependence upon a sudden connection of the bias potential. The quasi-steady-state regime is preceded by a transient regime, which last for a time proportional to the length of the central sample, and followed by recursions, at times proportional to the leads' size. Superimposed on the quasi-steady-state, we also observe finite-size current oscillations, whose behaviour depends crucially on the initial state of the system. I will finish by showing how a time-resolved Kubo formula is able to reproduce the emergent Landauer transport regime, as the leads size increases. These predictions may be of interest to future experiments on transport of fermionic ultra-cold atoms in optical lattices [3,4]

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Acknowledgements:
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List of Posters participating in Best Poster Award[1]

Code	Poster
PA01	**Measuring the spectral properties of the skin of human faces** Dora N. Marques, João M. M. Linhares, Andreia E. Gomes, Ricardo J. F. Pereira, Sérgio M. C. Nascimento
PA02	**Best daylighting for viewing the skin of human faces** Andreia E. Gomes, João M. M. Linhares, Ricardo J. F. Pereira, Sérgio M. C. Nascimento
PA03	**Exciton-polaritons in a cylindrical microcavity with an embedded 2D semiconductor layer** José Nuno S. Gomes, Carlos Trallero-Giner, Nuno M. R. Peres, Mikhail I. Vasilevskiy
PA04	**Optical Kerr effect in graphene under pulsed illumination in the visible spectral range** Diogo Cunha, César R. Bernardo, Michael Belsley, Mikhail Vasilevskiy
PA05	**Excitation of Graphene Plasmons by Quantum Emitters** Beatriz Ferreira, Nuno Peres
PA06	**The versatility of membrane-water partitioning in pharmacokinetic modelling** Eduarda Fernandes, T. Soares, A. Almeida, S. Benfeito, C. M. Lopes, B. Sarmento, F. Borges, M.E.C.D. Real Oliveira, M. Lúcio
PA07	**Liposomal Curcumin to overcome multidrug resistance in Cancer Treatment** Telma B. Soares, A. Dias, M.E.C.D. Real-Oliveira, M. Lúcio
PA08	**Liposomal hydrogels for the intravaginal co-delivery of antiretroviral drugs** Maria J. Faria, M. E. C. D. Real Oliveira, J. das Neves, T. Viseu and M. Lúcio
PA09	**Lipid colloidal dispersions loaded with omega-3 fatty acids and/or resveratrol developed for topical application against psoriasis** Ana R. Caldas, M.E.C.D. Real Oliveira, C. M. Lopes and Marlene Lúcio
PA10	**Plasmonic magnetogels as composite systems for multimodal cancer therapy** Sérgio R. S. Veloso, Paula M. T. Ferreira, J. A. Martins, Paulo J. G. Coutinho, Elisabete M. S. Castanheira
PA11	**PEGylated magnetoliposomes based on calcium-substituted magnesium ferrite nanoparticles as curcumin nanocarriers for cancer therapy** Beatriz D. Cardoso, A. Rita O. Rodrigues, B. G. Almeida, P. J. G. Coutinho, Elisabete M.S. Castanheira
PA12	**Synthesis and characterization of magnetoliposomes containing nickel ferrite nanoparticles covered with gold for applications in phototherapy** Irina S. R. Rio, Ana Rita O. Rodrigues, Elisabete M. S. Castanheira, Paulo J. G. Coutinho
PA13	**Development of magnetic nanoparticles decorated with silver for photodegradation of textile dyes with visible light** Ricardo J. C. Fernandes, Carlos A.B. Magalhães, Carlos O. Amorim, Vítor S. Amaral, Bernardo G. Almeida, Elisabete M.S. Castanheira, Paulo J.G. Coutinho
PA14	**Formation of monoolein-cationic lipid nanoparticles by solvent-exchange in bulk and microfluidics** Margarida M. Barros, C.J.O. Ferreira, M.E.C.D. Real Oliveira1 B.F.B. Silva

1 Posters will be on display in the Hall of CPII building. The selected flash presentations will be delivered in the Auditorium B2 of CPII building

PA15	**Simulation of the temperature profile of $BaCaZrTiO_3$ thin films during laser annealing** Tiago Rebelo, Bernardo G. Almeida
PA16	**Multiferroic $CoFe_2O_4$\$LiNbO_3$ Bilayers** Bruna M. Silva, J. Oliveira, J.A. Mendes, B.G. Almeida
PA17	**Chromium triiodide magnetic nanofibers** Vahideh Bayzi Isfahani, João H. Belo, Loukya Boddapati, Anabela Gomes Rolo, Rosa M. F. Baptista, Leonard Francis, João P. Araújo, Etelvina de Matos Gomes, Bernardo Almeida
PA18	**High-quality graphene-based dispersions for flexible electronics** Miguel Monteiro, Sergey Tkachev, Andrea Capasso, Pedro Alpuim
PA19	**Two-dimensional MoSe2 growth on soda-lime glass by chemical vapor deposition** João N. Rodrigues, J. Santos, P. Alpuim, A. Capasso
PA20	**Towards graphene based RF devices** Vitor Silva, I. Colmiais, L. Baptista, J. Borme, P. M. Mendes, P. Alpuim
PA21	**Label-free detection of DNA using graphene liquid-gate transistors** Telma Domingues, J. Rafaela Guerreiro, A. Ipatov, A. Purwidyantri, J. Borme, M. Prado, P. Alpuim
PA22	**Field-Effect Transistors as biosensors: building up for the end application** Patrícia D. Cabral, T. Rodrigues, J. Borme, E. Fernandes, P. Alpuim
PA23	**Au:CuO Nanocomposite Thin Films for Gas Sensing with High-Resolution Localized Surface Plasmon Resonance Spectroscopy** Manuela Proença, Marco S. Rodrigues, Joel Borges, Filipe Vaz
PA24	**Influence of a plasma treatment on the microstructure and plasmonic behaviour of Au-Al2O3 thin films** Diana I. Meira, Marco S. Rodrigues, Joel Borges, Filipe Vaz
PA25	**Influence of nanoparticle size and composition on the plasmonic response of Au-TiO_2 and Ag/Au-TiO_2 thin films** Diogo Costa, Marco S. Rodrigues, Lucian Roiban, Philippe Steyer, Joel Borges, Filipe Vaz
PA26	**Transparent Niobium-doped Titanium Dioxide Thin Films with high Seebeck coefficient for thermoelectric applications** Joana M. Ribeiro, Filipe C. Correia, Carlos J. Tavares
PA27	**Thermoelectric study of ZnO-based thin films: the effect of Bi dopant content** Filipe C. Correia, J.M. Ribeiro, J.S. Reparaz, A.R. Goñi, A.M. Mendes3 C.J. Tavares
PA28	**Water-based CuInxGa1-xSe2 chalcopyrite nanoink for flexible solar cells** Bruna F. Gonçalves, Viviana Sousa, Gabriela Botelho, Yury V. Kolen'ko, Senentxu Lanceros-Mendéz
PA29	**Water-based graphene inks for printed electronics** Miguel Franco, Raquel Alves, Pedro Costa, Senentxu Lanceros-Méndez
PA30	**Mechano-electrical skeletal muscle cell stimulation for tissue regeneration** Sylvie Ribeiro, C. Ribeiro, E. O. Carvalho, C. R. Tubio, N. Castro, N. Pereira, V. Correia, A. C. Gomes and S. Lanceros-Méndez
PA31	**High magnetoelectric response materials for all-printed electronics** Ana C. Lima, N. Pereira, R. Polícia, C. Ribeiro1, V. Correia, S. Lanceros-Mendez, P. Martins
PA32	**Evaluation of the bacterial response to piezoelectric microenvironments** Estela O. Carvalho, Margarida M. Fernandes, Jorge Padrao, Ana Nicolau, Jorge Marqueś-Marchań, Agustina Asenjo, Francisco M. Gama, Clarisse Ribeiro, Senentxu Lanceros-Mendez

PA33	**Thermochromic and Thermoresistive Ionic Liquids based Printable Materials** Liliana Correia Fernandes, Daniela Maria Correia, Clara García-Astrain, Nelson Pereira, Mohammad Tariq, José M. S. S. Esperança and Senentxu Lanceros-Mendez
PA34	**Development of magnetoelectric materials for printed electronics** Nelson Pereira, A. C. Lima, R. Polícia, V. Correia, P. Martins and S. Lanceros-Mendez
PA35	**Micropatterned electroactive polymers for biomedical and energy applications** Teresa Marques-Almeida, R. Gonçalves, S. Ribeiro, D. Miranda, M. M. Silva, V. F. Cardoso, F. M. Gama, C.M. Costa, C. Ribeiro, S. Lanceros-Mendez
PA36	**Ionic-Liquid-Based Electroactive Polymer Composites for MuscleTissue Engineering** Rafaela M. Meira, D. M. Correia, S. Ribeiro, P. Costa, A.C. Gomes, F.M. Gama, S. Lanceros-Méndez and C. Ribeiro
PA37	**Nano and micro materials for highly efficient arsenic removal from water** Hugo Salazar, P. M. Martins, Kiran P. Shejale, Rakesh K. Sharma, R. Krishnapriya, S. Ferdov, M. Silva, G. Botelho, A. Fidalgo-Marijuana and S. Lanceros-Mendez
PA38	**Surface engineering of nanostructured Ta surface with incorporation of osteoconductive elements by anodization** Luísa Fialho, Sandra Carvalho
PA39	**Alternative coatings to hexavalent chromium in applications under cyclic loads** Edgar Carneiro, José D. Castro, S. Carvalho
PA40	**Multifunctional coatings based on doped Ag-TiN for 3D printed ceramic pieces** José D. Castro, E. Carneiro, S. M. Marques, Bruno Figueiredo, Antonio J. Pontes, Álvaro M. Sampaio, Isabel Carvalho, Mariana Henriques, Paulo J. S. Cruz, S. Carvalho
PA41	**TiSiN(Ag) coatings deposited by HiPIMS** Diogo Cavaleiro, F. Fernandes, S. Carvalho
PA42	**Oxidation of Metallic and Bimetallic Nanoparticles Produced by Magnetron Sputtering** Hafsae Lamsaf, L. Rebouta, S. Carvalho, S. Calderon V.
PA43	**Effect of morphology on the wear behaviour of CrN coating deposited by arc-PVD method** Rita Ferreira, Óscar Carvalho, Luís Sobral , Sandra Carvalho, Filipe Silva
PA44	**A Polynomial Approach to the Spectrum of Dirac-Weyl Graphene Flakes** Maurício F. C. M. Quintela, João M. B. Lopes dos Santos1
PA45	**Edge-magnetism in Transition-metal Dichalcogenide Nanoribbons** Francisco M. O. Brito, João M. V. P. Lopes, Eduardo V. Castro

Measuring the spectral properties of the skin of human faces

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Keywords: Spectral properties, human skin, contact spectrophotometer, telespectroradiometer, hyperspectral imaging

Abstract: Measuring the spectral properties of the human skin is important as the spectral information may provide further detailed information than RGB data alone (Hughes et al., 2004; Nishidate et al., 2013).
Traditional methods are based on contact spectrometers that provide only information of a given area at a time, hindering comparisons among different areas or successive measurements.
This work aimed at obtaining the spectral properties of the skin of human faces using three different methodologies and analysing their differences.
Three instruments were used in six participants: a contact spectrophotometer (SPM, 400-700nm, 10nm steps), a telespectroradiometer (TSR, 380-780nm, 4nm steps) and a Hyperspectral Imaging System (HIS, 400-720nm, 10nm steps; spatial resolution of 1024(V)x1344(H) pixels. The spectral reflectance was estimated in each case. The similarity index (SI) (Wan et al., 2002) and the CIEDE colour difference formula in the CIELAB colour space assuming the CIE E illuminant and the CIE 1931 standard observer (CIE, 2004) were estimated. The reflectance measured with the SPM was assumed as the ground truth.
The SI and the chromatic difference of the TSR and the HIS compared against the SPM were of 85% and 80% and 4.4(±1.8) and 4.6(±2.3), respectively.
These results seem to suggest that the TSR and the HIS seem to provide good spectral accuracy when compared with traditional methods (SPM). They also seem to indicate that the HIS seems to be a capable tool for providing valuable spectral information of the human skin, in particular by combining the spatial and the spectral information.

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Best daylighting for viewing the skin of human faces

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Keywords: skin color; illumination; visual perception; psychophysics; hyperspectral imaging

Abstract: The color of the human skin provides several types of information about the individual [1,2]. As the perception of the human skin is influenced by the color and spectrum of the illumination it is important to estimate the light that observers prefer to visualize natural human skin. The purpose of this work was to estimate the best daylight illumination for viewing the skin of human faces. Eleven hyperspectral images from human faces were imaged and the reflectance spectra estimated. Spectral radiance was then computed assuming daylight illuminants from 4000K to 25000K in 41 steps and the tristimulus values were estimated assuming CIE1931 standard observer. Images obtained were then displayed in a CRT color monitor calibrated in color and luminance at 1m from the observer with an average luminance of 9 cd/m2. The observers' task was to select the images that produced the best visual impression. Seventeen young observers with normal color vison performed this experiment. The frequency of daylight illuminant selection was pooled across observers and a gaussian function was fitted to the data. The position of its maximum was assumed to be the preferred lighting condition. It was found that the preferred daylight illuminant had a CCT around 5310K, 5515K and 5215K for all, Black and White faces tested, respectively. These results seem to suggest that these observers preferred a smaller CCT when compared with the average daylight D65 and there are differences if Black and White skins are considered independently.

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Acknowledgements: This work was supported by the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2019.

Exciton-polaritons in a cylindrical microcavity with an embedded 2D semiconductor layer

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Keywords: exciton, Transition Metal Dichalcogenide, microcavity polariton, quantum emitter

Abstract: We describe exciton-polariton modes formed by the interaction between excitons in a nearly two-dimensional (2D) layer of a transition metal dichalcogenide (TMD) embedded in a cylindrical microcavity and the microcavity photons. For this, an expression for the excitonic susceptibility of a 2D semiconductor disk placed in the symmetry plane perpendicular to the axis of the microcavity is derived using second order perturbation theory. Using it, classical electrodynamics provides dispersion relations for the polariton modes, while the quantum-mechanical treatment of a simplified model yields the Hopfield coefficients [1] that measure the degree of exciton-photon mixing in the coupled modes. The density of states (DOS) and its projection onto the photonic subspace are calculated taking monolayer MoS2 embedded in a silica cylinder as an example. The calculated results demonstrate enhancement of the local DOS (Purcell effect [2]) for some values of angular momentum (μ), caused by the presence of the 2D layer. The effect is stronger than in a planar cavity that has been considered before. [3]

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Acknowledgements: Funding from the European Commission, within the project "Graphene-Driven Revolutions in ICT and Beyond" (Ref. No.696656), and from the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2013 is gratefully acknowledged.

Optical Kerr effect in graphene under pulsed illumination in the visible spectral range

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Keywords: graphene, pump-probe technique, optical Kerr effect, hot carriers

Abstract:

Pump probe spectroscopy is an experimental technique used to study ultrafast electron dynamics. In this work, a strong pump beam and, after a variable delay time, a weak probe beam were focused on a graphene layer deposited in a glass substrate. The pump beam excites free charge carriers of the material creating a non-equilibrium electronic distribution in the valence and conduction bands and the pump beam is used to observe the induced changes in the system by the pump beam. In the present work this technique was applied on the graphene using visible pulsed radiation (λ=400 nm). The application of a second beam, also in the visible region, with a wavelength deviated from 400nm, revealed a variation in the refractive index induced by the first beam, the optical Kerr effect. The effect is larger than what has previously been measured for graphene, in the visible spectral range [1].
The theoretical part of this work is dedicated to the explanation of the experimental results obtained. Once out-of-equilibrium due to the incidence of the pump beam the electrons start relaxing their energy through inelastic scattering processes interacting with lattice phonons. This relaxation is studied using the Fokker-Planck's equation, which allows to obtain theoretical expressions for the non-equilibrium charge carriers distribution. With this distribution, it is possible to calculate the perturbed graphene's optical conductivity and to explain theoretically the observed nonlinear optical effect.

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Excitation of Graphene Plasmons by Quantum Emitters

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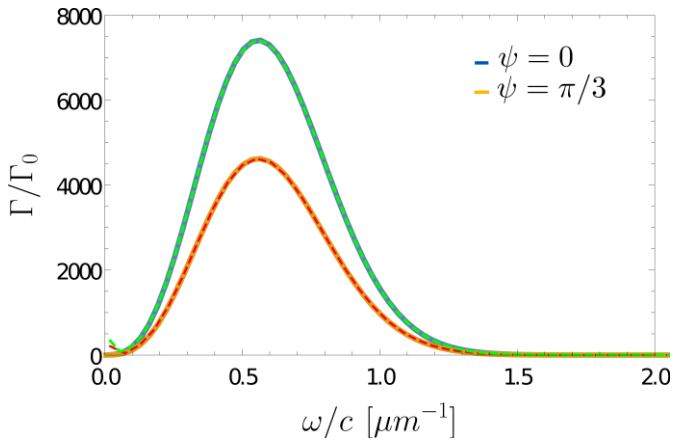
Keywords: Graphene, Plasmons, Quantum Emitters, Quantization

Abstract: In this work we show that is possible to excite plasmons in different graphene structures by simply placing a quantum emitter near the structure. We calculate the transition rate of the spontaneous decay of the emitter using the full EM dyadic Green's function. As an alternative to this, we introduce the macroscopic quantization of plasmons and calculate the transition rate using the quantized form of the electric field. With the two transition rates we can compare the classic case with the quantum emission one and we show that we obtain the same results.



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The versatility of membrane-water partitioning in pharmacokinetic modelling

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Keywords: Derivative spectroscopy; lipid nanosystems; pharmacokinetic profiling; membrane-water partition.

Abstract: In a rational drug design, the modulation of the chemical structure based on drug's pharmacokinetic profile can be the solution to avoid bigger investments in non-promising drugs. Numerous significant correlations between lipophilicity and membrane permeation have been established[1]. Additionally, anisotropic membrane-like systems, such as membranes/water (M/W) partitioning systems, are increasingly described as an alternative to octanol/water for the estimation of pharmacokinetic behaviour[2]. Actually, lipophilicity measured in isotropic octanol/water system only expresses the balance of hydrophobic and polar interactions. However, lipophilicity is the net result of all intermolecular forces, and when measured in the M/W systems, it also considers the ionic bounds, providing a better correlation with the intermolecular forces operating in molecular pharmacology and biochemistry[1]. In the present study, derivative spectroscopy was used to calculate M/W partition coefficient of drugs and to predict several parameters of their pharmacokinetic profile using lipid nanosystems of different constitution as biomembrane mimetic models [3]. Acyclovir, with *LogM/W*=3.05±0.06, showed tendency to be retained in *Stratum Corneum* after topical administration. For camptothecin, the partition in two models (*target* and *off-target* tissues) resulted in a higher value for *off-target* model. *LogM/W* of a newly-synthesized drug was determined in a biomimetic model of blood-brain barrier, in which the drug showed ability to reach its therapeutic target. The gastro-toxicity of Diclofenac was explained based on the interaction of this drug with relevant lipid membrane phases[4]. The results obtained highlighted the relevance of determining the *LogM/W* in biomimetic models to obtain reliable information in the early stages of drug development.

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Liposomal Curcumin to overcome multidrug resistance in Cancer Treatment

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Keywords: ADME profiling; Biophysical techniques; Cancer treatment; Lipid nanocarriers.

Abstract: Despite the long history of classical therapy improvement in cancer therapy, treatment failure is still frequently encountered. To overcome such failure researchers have focus onto new strategies for the prevention of cancer MDR, having natural compounds (i.e. polyphenols) emerged as an exciting solution mainly due to their chemosensitizer activity [1,2]. Within polyphenols sources, *Curcuma* genus has acquired significance due to the presence of curcumin, a compound with anti-inflammatory and antioxidant properties, recognised as valuable for cancer treatment [2].
In this work, using derivative spectroscopy; quenching of intrinsic fluorescence of human serum albumin; dynamic and electrophoretic light scattering, differential scanning calorimetry and small and wide angle x-ray diffraction, curcumin revealed low bioavailability, bioaccumulation, high affinity to plasma proteins, as well as a tendency to induce membrane biophysical changes, highlighting the need of delivery curcumin using nanocarriers.
Thus we develop lipid nanocarriers of Dimethyldioctadecylammonium bromide:monoolein(1:2) to load curcumin and both *C. longa* and *C. aromatica* extracts. The developed nanocarriers showed an encapsulation efficiency of approximately 100%, sizes lower than 200 nm, high stability when stored and a positive superficial charge. Moreover, an *in vitro* biphasic controlled release, of 94,5% of curcumin (R^2=0.998) after 50 h was observed and the ability to prevent interactions with plasma proteins, after successful PEGylation was proved. As final remark, the formulations developed herein confirmed the antioxidant activity of the encapsulated natural compounds by: (i) fluorescence decay of a lipophilic probe (DPH-PA) under the action of a peroxyl radical generator (AAPH) and (ii) COX-I inhibition by fluorescence.

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Acknowledgements: Funding for this work was provided by Fundação para a Ciência e Tecnologia (FCT) in the framework of the Strategic Funding UID/FIS/04650/2019 and in the ambit of the project CONCERT (POCI-01-0145-FEDER-032651 and PTDC/ NAN-MAT/326512017), co-financed by the European Regional Development Fund (ERDF), through COMPETE 2020, under Portugal 2020, and FCT I.P. T.B. Soares acknowledges FCT for the PhD grant with the reference SFRH/BD/138678/2018. M. Lúcio thanks FCT and ERDF for doctoral position [CTTI-150/18-CF(1)] in the ambit of the project CONCERT. The authors thank ELETTRA, Trieste, Italy, for beam time and support through the project 20155321.

Liposomal hydrogels for the intravaginal co-delivery of antiretroviral drugs

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Keywords: microbicide, liposomes, hydrogel, tenofovir disoproxil fumarate, emtricitabine

Abstract: The human immunodeficiency virus (HIV) stands as an increasing global burden and new strategies to control the viral transmission are critical. [1] Thus, we propose the development of a novel topical microbicide based on the commercial formulation Truvada®. Concretely, liposomes loaded with tenofovir disoproxil fumarate (TDF) were incorporated in carbomer-based hydrogels (HG) with emtricitabine (FTC) resulting in a final liposomal hydrogel for vaginal administration. [2]

To select the most suitable dosage forms, a rational approach comprising both pre-formulation and formulation studies was followed. Pre-formulation studies included *in silico* analysis of TDF/FTC as well as their interaction with lipid membranes. The interaction between mucin and different surface charged liposomes was also evaluated. Formulation studies included a thorough characterization of several lipidic compositions and encapsulation processes. The pharmaceutical performance of the formulation was predicted *in vitro* by studying: (i) the release profile of both drugs; (ii) TDF permeation; (iii) rheological profile and (iv) cytotoxicity.

After studying interactions with mucin, zwitterionic liposomes with mean diameter of 134 ± 13 nm and a transition temperature of 41 ºC were selected, demonstrating enhanced mobility properties. Additionally, liposomal formulations did not induce cellular toxicity and presented high encapsulation efficiencies (≈ 84%) for TDF, improving its permeation (J_{ss}=9.99 µg/cm^2/h). Drug loaded hydrogels displayed sustained release profiles for both TDF and FTC (≈ 60% after 7 h). Furthermore, liposomal hydrogels maintained suitable pseudoplastic profiles for vaginal administration. The obtained data support that the proposed liposomal hydrogels constitute a promising approach for the intravaginal co-delivery of TDF and FTC.

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Lipid colloidal dispersions loaded with omega-3 fatty acids and/or resveratrol developed for topical application against psoriasis

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Keywords: Psoriasis; omega-3; resveratrol; lipid nanosystems; semi-solid base.

Abstract: Psoriasis is an inflammatory and autoimmune skin disease with a high impact on patients' life. Conventional psoriasis therapies have several limitations, requiring new strategies (novel delivery systems and/or bioactive compounds) to improve therapeutic efficacy and reduce adverse effects[1,2]. It has been reported that resveratrol (RSV) or omega-3 fatty acids (ω3), have anti-inflammatory and immunomodulatory effects, justifying their use in psoriasis[1,3]. Thus, the objective of this work was to develop and optimize a topical semisolid formulation containing ω3 encapsulated in nanostructured lipid carriers (NLC) and liposomes, and RSV encapsulated in liposomes, for psoriasis. Ultrasound and hydration of the lipid film were the techniques applied to develop NLC and liposomes, respectively. The formulations were physical-chemically characterized to evaluate size, surface charge, encapsulation efficiency and shelf stability. Subsequently, the therapeutic performance of the formulations was predicted by *in vitro* assays to evaluate: the release profile of RSV; the anti-inflammatory/immunomodulatory effects regarding inhibition of COX-1/nitric oxide production; and the antioxidant effect. Finally, to allow better skin applicability, the selected formulations were incorporated into a hydrogel and evaluated regarding its rheological properties, occlusion potential and permeation capacity of loaded RSV. The formulations developed were stable and presented acceptable values of size and polidispersivity for topical application in psoriatic skin. Therapeutic performance studies highlighted properties relevant to the psoriasis treatment: 80 % release of RSV in 35 h, increased RSV permeability; anti-inflammatory/immunomodulatory effects and antioxidant capabilities. Furthermore, the hydrogel loaded with the formulation exhibited a pseudoplastic behaviour, favourable for the intended administration.

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Plasmonic magnetogels as composite systems for multimodal cancer therapy

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Keywords: Magnetogels; plasmonics; core/shell nanoparticles; gold-decorated nanoparticles; cancer therapy

Abstract: Conventional chemotherapeutic strategies have lack of specificity, therapeutic effectiveness and are expensive, besides worsening patient's quality of life. Supramolecular magnetogels are highly promising for biomedical applications such as magnetic resonance imaging, biosensing, hyperthermia and drug delivery [1,2]. The combination of hydrogels with plasmonic/magnetic nanoparticles affording plasmonic magnetogels allows the application of complementary strategies [3]. In this work, plasmonic magnetogels comprising two different plasmonic/magnetic nanoparticles architectures (core/shell and gold-decorated nanoparticles) were developed and characterized. Fluorescence-based techniques were used to assess hydrogelator physicochemical properties and incorporation of curcumin in the magnetogels, drug transport towards model membranes and controlled release. The gels showed to be suitable nanocarriers for this model antitumor drug, exhibiting reversible photothermia capabilities (Figure 1) and tuneable drug release. The magnetogels bearing gold-decorated nanoparticles showed the best photothermia properties [3].

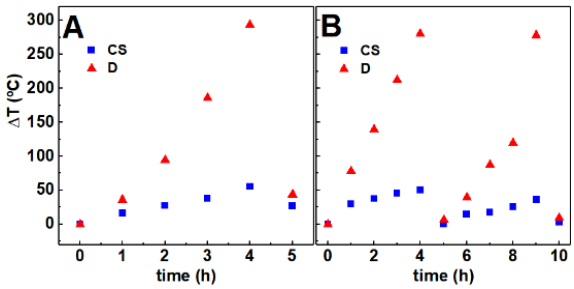

Figure 1. Temperature variation through irradiation of curcumin-loaded magnetogels containing core/shell manganese ferrite/gold nanoparticles (CS) and gold-decorated manganese ferrite nanoparticles (D). (A) First irradiation cycle. (B) Subsequent cycles of 5 hours.

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PEGylated magnetoliposomes based on calcium-substituted magnesium ferrite nanoparticles as curcumin nanocarriers for cancer therapy

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Keywords: Magnetoliposomes, cancer therapy, drug nanocarriers, curcumin, PEG

Abstract: Calcium-substituted magnesium ferrite nanoparticles ($Ca_xMg_{1-x}Fe_2O_4$, x=0.75, 0.25, 0.50) were synthesized by coprecipitation method and characterized on their colloidal stability and optical, magnetic and structural properties. Their superparamagnetic properties, biocompatibility and stable behaviour in aqueous solution make them suitable to be encapsulated into liposomes (aqueous magnetoliposomes – AMLs) or to be covered with a lipid bilayer (solid magnetoliposomes – SMLs). The resulting magneto-sensitive liposomes have the ability to encapsulate hydrophobic drugs, as the potential antitumor drug curcumin, and present an average hydrodynamic size of 150 nm with a reduced polydispersity index, following previous developed work [1]. To reduce *in vivo* opsonisation ensuring that liposomes are not rapidly cleared by mononuclear phagocyte system, sterically stabilized liposomes were developed. Strands of polyethylene glycol (PEG), a highly hydrophilic polymer, were attached to magnetoliposomes surface via a cross-linked lipid in a process known as PEGylation. The ability of the PEGylated and non-PEGylated nanosystems to interact with biological membrane models (giant unilamellar vesicles) was evaluated by Förster resonance energy transfer (FRET) or fluorescence quenching assays. The influence of an alternating magnetic field (AMF) on drug release from magnetoliposomes over time was evaluated and compared with curcumin release by diffusion at the same time intervals. These results suggest the potential of drug-loaded PEGylated magnetoliposomes as nanocarriers that can be magnetically guided to the tumor sites and can act as agents for a synergistic approach combining magnetic hyperthermia and chemotherapy in a single system (Figure 1).

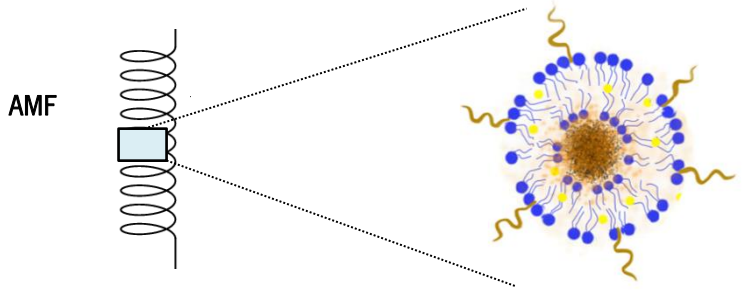

Figure 1: Schematic representation of a PEGylated magnetoliposome releasing the encapsulated payload (curcumin) upon the stimulus of an alternating magnetic field (AMF).

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Synthesis and characterization of magnetoliposomes containing nickel ferrite nanoparticles covered with gold for applications in phototherapy

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Keywords: Phototherapy, magnetic/plasmonic nanoparticles, nickel ferrite, gold nanoparticles, magnetoliposomes

Abstract: Currently, cancer is one of the leading causes of death worldwide. Despite the investigations and discoveries to date, there are many difficulties in rapid diagnosis, as well as in targeted treatments to reduce side effects. Nanotechnology has increasingly allowed the development of new techniques and strategies for application in cancer therapy, for example, using hyperthermia. Magnetic nanoparticles have been increasingly important in this regard, due to their unique characteristics, such as the ability to target a specific therapeutic site using external magnetic field gradients. On the other hand, gold has been used in different applications, from particle coating to prevent agglomeration, to the use of gold nanoparticles for local heating in cancer therapy. In this work, nanoparticles with magnetic/plasmonic properties of nickel ferrite decorated with gold nanoparticles and core/shell nickel ferrite/gold nanoparticles were prepared and characterized. The synthesized nanoparticles were used for the preparation of solid magnetoliposomes (SMLs), these systems being our target of study. The nanosystems were evaluated for the ability to cause local heating upon excitation in the gold plasmonic band. For that, fluorescence quenching of rhodamine B incorporated in SMLs lipid layer was measured [1]. The developed multifunctional nanosystems have shown promising results for application in combined cancer therapy (chemo/phototherapy).

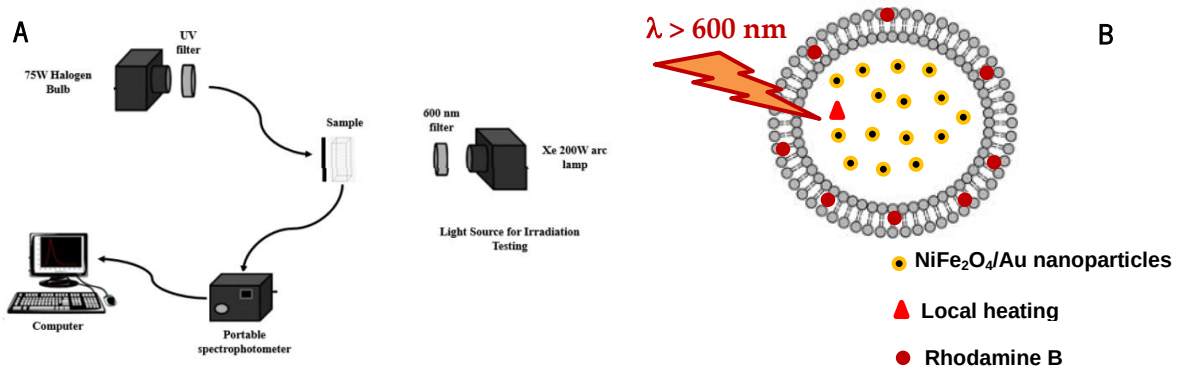

Figure 1. A: Irradiation setup. **B:** Schematic representation of local heating, by action of the covered gold nanoparticles.

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Development of magnetic nanoparticles decorated with silver for photodegradation of textile dyes with visible light

Ricardo J. C. Fernandes[1]*, Carlos A.B. Magalhães[1]*, Carlos O. Amorim[2], Vítor S. Amaral[2], Bernardo G. Almeida[1], Elisabete M.S. Castanheira[1], Paulo J.G. Coutinho[1]

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Keywords: ferrites, visible light, photocatalytic activity, dyes

Abstract: Magnetic nanoparticles of zinc/calcium ferrite decorated with silver exhibit promising results towards photodegradation of dyes. The band gap of these mixed ferrites, 1.78 eV, allows the use of visible light in the photocatalytic process. The partial substitution of zinc by calcium in ferrite structure increases biocompatibility and magnetic behavior. On the other hand, the presence of silver decreases the recombination rate of electrons and holes, enhancing the photocatalytic activity.

In this work, zinc/calcium ferrite nanoparticles decorated with silver were synthesized by coprecipitation method. The nanoparticles were characterized by XRD, UV/Vis absorption, TEM and SQUID. The photodegradation potential was assessed with a model dye (Rhodamine B) and industrial textile dyes (CI Reactive Red 195, CI Reactive Blue 250 and CI Reactive Yellow 145) [1]. The results showed a high photocatalytic activity using visible light (figure 1), as well as magnetic properties that allow the recovery and reutilization of the nanoparticles. These properties are important in both economic and environmental terms, being a step towards a sustainable and efficient photoremediation of industrial textile effluents.

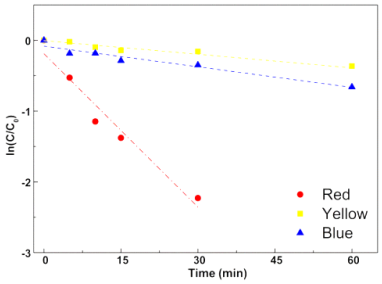

Figure 1. Plot of the pseudo-first-order kinetics for degradation of textile dyes. Red: CI Reactive Red 195; Blue: CI Reactive Blue 250; Yellow: CI Reactive Yellow 145.

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Formation of monoolein-cationic lipid nanoparticles by solvent-exchange in bulk and microfluidics

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Keywords: monoolein; cationic lipids; solvent-exchange; microfluidics

Abstract: Tuning the sizes of lipid nanoparticles is an important capability when designing drug/gene delivery formulations. Recently, we proposed the use of microfluidics to tune the sizes of monoolein (MO)[1],[2] nanoparticles. This control is achieved via manipulating the flow-rate ratio between an ethanolic solution carrying MO and two aqueous side-streams, squeezing the ethanol and promoting mixing with water[3]. This leads to the formation of MO nanoparticles in a controlled way. The higher the flow-rate ratio, the smaller the NPs.
In this work, we explore the effect of adding a cationic lipid (Cat.Lip.-DDAB/DODAB) to MO-nanoparticles with the goal of embedding cationic charge on the particles and making them suitable to encapsulate nucleic acids[4]. Interestingly, we observe that the addition of even minute quantities of Cat.Lip (0.01%) strongly shifts the assembly behaviour. Whereas in neat MO, the NPs sizes can be tuned with the flow-rate ratio in the microfluidic devices, in Cat.Lip:MO systems, the final particle size becomes independent of rate flow conditions and markedly smaller. By performing this solvent-exchange Cat.Lip:MO NP formation in bulk conditions, similar sizes to the ones from microfluidics are observed, contrary to the neat MO system. This leads us to believe that in the presence of Cat.Lip. the rate-limiting step for NP formation is not mixing any longer, but rather the formation and/or stabilization of an intermediate structure, such as bilayer disks. The small sizes observed also suggest that the final NPs structure is not cubosomes. Cryo-TEM observations are being planned to validate these hypotheses.

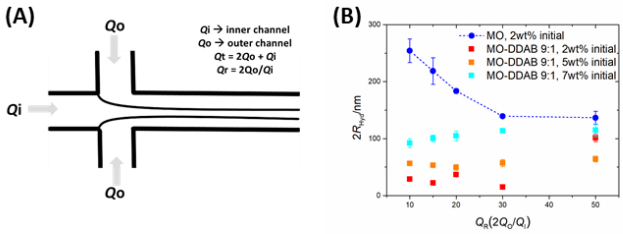

Figure 1. (A) Schematization of the hydrodynamic focusing flow. (B) Hydrodynamic diameter (2RHyd) dependence of MO and MO-DDAB formulations as a function of the flow rate ratio Q_R.

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Acknowledgements: This research is supported by Microfluidic Layer-by-layer Assembly of Cationic Liposome - Nucleic Acid Nanoparticles for Gene Delivery project (032520) co-funded by FCT and the ERDF through COMPETE2020.

Simulation of the temperature profile of $BaCaZrTiO_3$ thin films during laser annealing

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Keywords: thin films, annealing, temperature, simulation, crystallinity

Abstract: Multiferroic piezoelectric-magnetostrictive composites represent great interest due to the coupling of electric/magnetic responses. In this respect, in composite nanostructures of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ (BCZT, ferroeletric) thin films on metglas substrates (ferromagnetic), the BCZT has to be deposited at low temperatures to avoid substrate damage. However, thin films deposited at low temperatures exhibit a high density of defects and low crystallinity. Additionally, in the BCZT/metglas case, annealing in a conventional oven can't be done since it would degrade the substrate. An alternative is performing a pulsed laser annealing, minimizing the heated region and the degradation of the metglas. The simulation of the annealing process is then useful to understand how its parameters (energy and fluence of the laser, pulse duration, etc) influence the optimization of the film's crystallinity. The BCZT film was prepared by laser ablation on a Metglas 2826MB substrate. A 248 nm KrF pulsed laser was used for both the ablation and the annealing. The temperature variation with the depth relative to the film's surface and on annealing time was then studied (Figure 1), using a 1D heat diffusion equation combined with a finite difference method. The laser intensity, BCZT's reflectivity and the temperature dependence of the thermal conductivity and specific heat of the BCZT were considered. No structural phase changes were detected in both the BCZT and the metglas for the values of laser fluence studied, but for 80 mJ/cm^2 the maximum temperature approached is near the BCZT's melting point. It was observed that since the film's thermal conductivity decreases with increasing fluence, lower fluences allow for a better distribution of the laser's energy throughout the crystal lattice, increasing the crystallinity. Furthermore, between consecutive pulses the film's temperature stabilizes at room temperature.

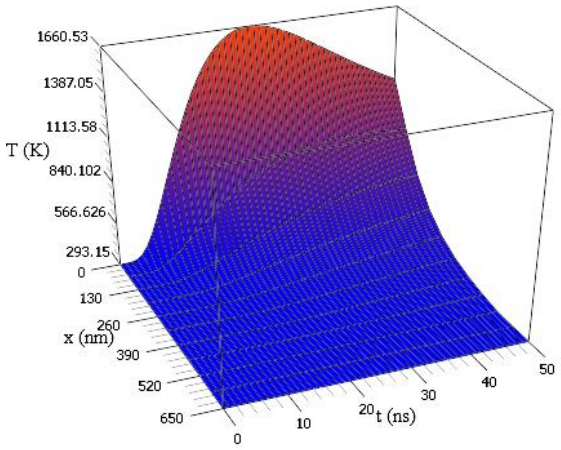

Figure 1. Temperature profile of the sample during one laser pulse

Multiferroic $CoFe_2O_4$\$LiNbO_3$ Bilayers

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Keywords: multiferroics bilayers, magnetoelectric effect, $CoFe_2O_4$\$LiNbO_3$

Abstract: Nanostructured multiferroic thin films constructed by combining magnetostrictive and piezoelectric materials have attracted recently much scientific and technological interest. In addition to possessing ferroelectricity and ferromagnetism in each individual phase, they are shown to exhibit stress mediated coupling between their magnetic and electric properties, called magnetoelectric effect. This coupling between their magnetic and electric degrees of freedom may then give rise to new physical phenomena and applications. Lithium niobate ($LiNbO_3$) is a ferroelectric material with good piezoelectric, pyroelectric, electro-optical, birefringent, photorefractive and photoelastic properties which are favorable towards applications. Cobalt ferrite ($CoFe_2O_4$) presents a high magnetocrystalline anisotropy and magnetostriction, making it suitable for application in magnetoelectric composite thin films. Here, bilayer composite thin films, composed by a $LiNbO_3$ layer deposited over a $CoFe_2O_4$ film have been prepared by laser ablation on platinum covered Si(001) substrates. Their structural, microstructural and dielectric properties were characterized. The X-ray diffraction measurements show a rhombohedral ferroelectric phase in $LiNbO_3$ and a cubic spinel structure in $CoFe_2O_4$. The SEM micrographs show dense films, with cobalt ferrite and lithium niobate layer thicknesses in the range 100-200nm and 400-800nm, respectively. Their dielectric properties were characterized by impedance spectroscopy. In order to obtain the relaxation times and activation energies, the electrical permittivity (figure 1) was fitted, using appropriate models for the behavior of the polarization and including a conductivity contribution. As such, the influence of the synthesis conditions on the dielectric properties of the films and their evolution with individual layer thicknesses, will be discussed.

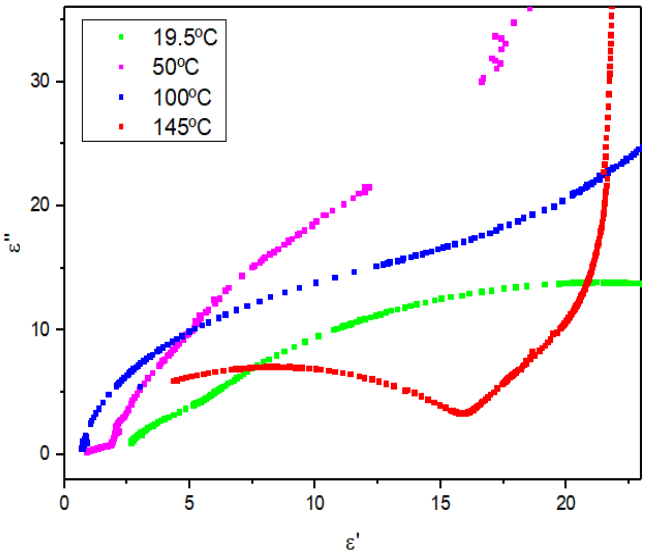

Figure 2: Imaginary component of electrical permittivity as a function of real component.

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Chromium triiodide magnetic nanofibers

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Keywords: Nanofibers, electrospinning, CrI_3, PEO, magnetic

Abstract: Low-dimensional semiconductor magnetic materials have been attracting much attention, due to their potential applicability in a wide range of technologies, such as data storage or sensing. In this respect chromium triiodide (CrI_3) is a van der Waals bonded layered semiconductor, which presents ferromagnetism for temperatures below 68 K, and the transition temperature can be tuned by an applied electric field. On the other hand, electrospinning is a low cost versatile method for producing fibers with diameters down to a few tens of nanometres. Then, by choosing suitable inclusions in the polymeric fibre matrix, their functionalization can be attained. Thus, the present study focuses on the fabrication and characterization of magnetic nanofiber mats composed of polyethylene oxide (PEO) and chromium triiodide. The samples were prepared by the electrospinning technique, for different concentrations, feeding rates and applied electric fields. The X-ray diffraction (XRD) analysis indicates that the nanofibers are composed by CrI_3 inclusions in the PEO matrix, with the CrI_3 hexagonal structure. Raman spectroscopy further shows the presence of the CrI_3 modes in the fibre mats. According to the FESEM images, the amount of CrI_3 particles in the precursor solutions directly affects the uniformity and diameter distribution of the fibres. The nanofiber samples containing less amount of CrI_3 are more uniform, with an average diameter of 460 nm. The magnetization of the samples as a function of temperature was characterized. The results indicate the presence of ferromagnetism below 51 K, superimposed with an antiferromagnetic phase. This feature was confirmed by M vs H isothermal hysteresis curves measured at different temperatures. As such, the magnetic behaviour of the samples and its correlation with the preparation conditions will be discussed.

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High-quality graphene-based dispersions for flexible electronics

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Keywords: printed electronics, conductive and transparent films, liquid phase exfoliation, TCO

Abstract: The development of graphene-based nanomaterials for flexible electronics is of high interest for the industry [1]. Liquid dispersions of these materials are suitable for the deposition of films with electrical conductivity, transparency, flexibility, low cost and compatibility with a wide range of substrates [2, 3]. To date, graphene-based dispersions are still rather expensive and present some limitations (*e.g.*, they require high-temperature post-processing, or have limited compatibility with substrates). Here, we propose a novel approach to produce graphene-based dispersions with high yield and control on the material properties. Our approach underpins on the use of shear mixing and ultra-sonication techniques for an effective milling and exfoliation of natural graphite into graphene flakes, suspended in different solvents. The samples were carefully characterized by dynamic light scattering, X-ray diffraction, scanning and transmission electron microscopy, and Raman spectroscopy.
By using a combination of shear mixing and ultra-sonication with tuned conditions (such as time, frequency, and power), we produced stable graphene dispersions with concentrations above 4 mg/mL (with lateral size of the graphene flakes between 30 nm and 500 nm). The dispersions can be deposited by several techniques (*e.g.*, spray coating, inkjet and screen-printing, etc.) on various substrates to fabricate films with desired levels of transparency and conductivity. In our tests, specific formulations for spray coating were prepared by mixing the graphene-based dispersions with polymeric additives. These formulations were used to spray-coat films on flexible PET and glass substrates, achieving an optical transmission (in the visible range) of 70-91% and a sheet resistance of 0.35-4 kΩ/□.

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Two-dimensional $MoSe_2$ growth on soda-lime glass by chemical vapor deposition

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Keywords: two-dimensional materials, transition metal dichalcogenides, optoelectronics

Abstract: Two-dimensional (2D) semiconductors are currently a topic of high interest in the materials science community. These materials, lightweight and flexible, show outstanding optoelectronic properties [1,2], such as thickness-dependent photoluminescence. Atomically thin MoS_2 and $MoSe_2$, in particular, have been proposed and applied in several electronic devices [3]. Notwithstanding this considerable effort, a production method that would guarantee large scale, high throughput and low cost is still lacking. Chemical vapor deposition (CVD) is seen as one of the most promising production methods for batch production of 2D semiconductors with high quality, but a few crucial challenges are still to be faced to attain a cost-effective and reproducible process for uniform samples over large areas.

In this work, we report the synthesis of 2D $MoSe_2$ by CVD on inert substrates (*i.e.*, soda lime glass and quartz), using selenium powder and molybdenum foil as solid precursors (Figure a). The samples were evaluated by electron and atomic force microscopy, as well as Raman and X-ray photoelectron spectroscopy. By tuning the process parameters, monolayer $MoSe_2$ film with large-area was grown on glass which showed intense photoluminescence at ~1.57 eV (Figure b). By comparing samples grown in the same conditions on the two different substrates, we ascertained that the presence of Na (originating from the glass substrate during CVD) has a key role in the process, promoting an extensive horizontal growth of the 2D film [4]. The 2D $MoSe_2$ samples can be integrated in optoelectronic devices, such as photodetectors, taking advantage of their high photo-responsivity.

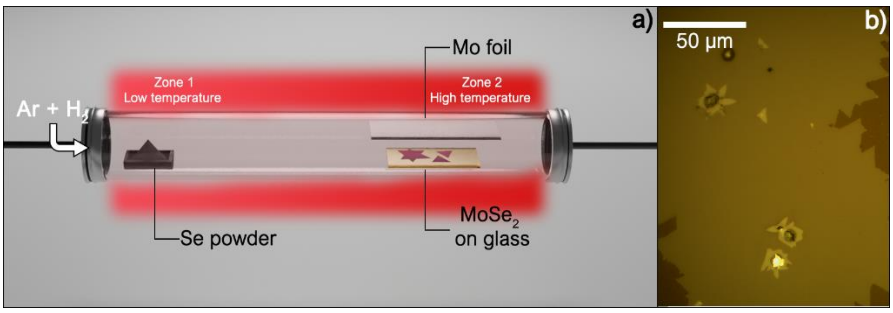

Figure. *a) Schematic of the CVD system; b) Optical image of monolayer $MoSe_2$ (bright area) grown on glass.*

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Towards graphene based RF devices

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Keywords: graphene, RF, transistors, inductors, capacitors

Abstract: Graphene has become a very attractive material due to its amazing properties. High carrier mobility, high carrier velocity saturation, high current density, and silicon compatibility make it suitable for radiofrequency (RF) applications. Reported graphene transistors can achieve intrinsic cut-off frequencies higher than 300 GHz [1]. This kind of transistors are very promising in applications for small-signal circuits (AC/RF) and are used in several RF applications such as RF oscillators, mixers and RF power amplifiers. To obtain such integrated devices it is still necessary to develop and include graphene inductors and capacitors.
Due to its high conductivity and large kinetic inductance, graphene can potentially increase the Q factor of inductors and their inductance density values (up to 1.5 times higher than its metallic counterpart). Such improvements ultimately reduce the total area of integrated circuits and improve their performance [2]. Graphene based varactors have also been proposed. In addition to their low tuning voltage and simplified fabrication process, their tunability range results in varactors with a capacitance that is 100 times larger than RF MEMS, and outperform MOSCAPs at higher frequencies [3]. Finally, it is of special interest to congregate the advantages of using graphene transistors and passive components to produce an RF circuit. In Figure 3, a graphene transistor is shown with a single core-shell nanowire gate, which is being developed in our group and is aimed to be integrated with passive graphene components.

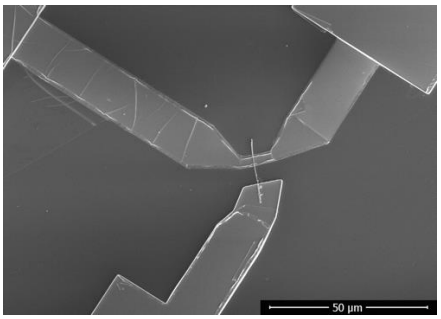

Figure 3 – SEM image of a graphene transistor with an aligned single core-shell nanowire gate.

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Label-free detection of DNA using graphene liquid-gate transistors

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Keywords: Biosensor, graphene, DNA, electrolyte-gate transistor

Abstract: In recent years, DNA detection platforms have developed at a dizzying pace as they provide information for a wide range of fields, including molecular biology research, genetic disease diagnosis, forensics and environmental monitoring. Graphene transistors (GFETs), offer the potential to perform rapid, label-free, and highly sensitive assays. This properties and the potential for integration into portable instrumentation makes GFETs appropriate for diagnostics. [1]
In this work we develop a miniaturized DNA sensing device, based on liquid-gate GFETs. The sensor readout consists of a home-made electronic platform, with the size of a credit card, to ensure portability. The GFET sensor chip and a PDMS flow cell, fitting the sensor layout, are assembled and then inserted in the portable platform (Fig. 1c,d). This system, connected to a syringe pump and a multiposition valve, allows for automation, improving the precision over manually operated ones [2].
For DNA detection, the GFET channel was functionalized with a probe (30 nucleotides, complementary to the target DNA) immobilized on the graphene by a heterobifunctional linker (PBSE) that covalently binds to the amine modified probe. To block unreacted ester groups of PBSE, ethanolamine is added before introducing the solutions containing the target molecules. Biorecognition events result in a positive gate voltage shift of the graphene charge neutrality point. The graphene transistor biosensor displays a sensitivity of 16.1 mV/dec with a limit of detection of ~4 aM. The sensor response in real time was studied during probe immobilization and target hybridization.

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Acknowledgements: This work was supported by projects POCI-01-0145-FEDER-031069 (FCT-PORTGRAPH) and ATTRACT grand agreement 777222 (H2020-MULTIMAL).

Field-Effect Transistors as biosensors: building up for the end application

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Keywords: Biosensors, EG-GFET, MOSFET, Protein biomarkers

Abstract: Biosensing requires a biorecognition and a transducing element, for the specific interaction with a particular biomolecular target, and for converting that chemical interaction into a measurable signal, respectively. In this work, two transducing models were explored: (1) standard gold electrodes were fabricated, functionalized for biorecognition, and connected to a commercial p-type MOSFET; (2) novel electrolyte-gated graphene field-effect transistors (GFETs) were fabricated and prepared for direct exposure of the biological media over the graphene channel. Both models were studied against biocompatible solutions at different ionic strengths to provide understanding of the mechanisms explaining the bio-detection system. To render the sensor surface suitable for specific biorecognition, the gold electrodes connected to the MOSFET were functionalized using a thiol-based linker, while the graphene channel of GFETs was modified using a pyrene-based linker that provides a stable and efficient interface for the development of the immuno-assay. Detection of a protein biomarker relevant for stroke patient stratification was achieved in both models. The functionalized devices were exposed to cellular Fibronectin at concentrations ranging from 0.5 to 5 μg/mL, corresponding to the clinically relevant range of the biomarker. The results show that the MOSFET-based system provides improved signal stability during acquisition, however it is less sensitive to the biointerface making interpretation of the bio-interface events problematic. The GFET system, although less stable, provides consistent behaviour related to the biointerface, being possible to correlate the signal variation with the steps of surface modification and with the biomarker detection at different concentrations.

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Au:CuO Nanocomposite Thin Films for Gas Sensing with High-Resolution Localized Surface Plasmon Resonance Spectroscopy

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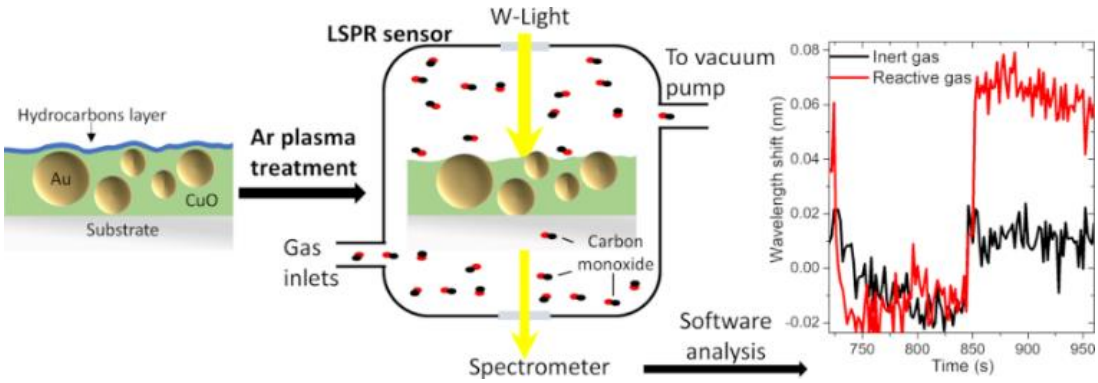
Keywords: Thin films; Gold Nanoparticles; Localized Surface Plasmon Resonance; Gas Sensing

Abstract: Gas sensing, based on bulk refractive index (RI) changes, has been a challenging task for localized surface plasmon resonance (LSPR) spectroscopy, as demonstrated by the very limited bibliography available in this field [1,2]. In this work, it is demonstrated that a plasmonic thin film composed of Au nanoparticles embedded in a CuO matrix can be used to detect small changes (as low as 6×10^{-5} RIU) in bulk RI of gases at room temperature, using a High-Resolution LSPR spectroscopy system. Such thin film system was optimized by reactive magnetron sputtering, followed by an in-air annealing protocol treatment at 700 ºC to promote the Au nanoparticles growth [3]. To enhance the film's surface activity, a simple Ar plasma treatment revealed to be enough to remove the top monolayers of the film and to partially expose the embedded nanoparticles, and thus promoting the film's gas sensing. The treated sample exhibit high sensitivity to inert gases (Ar, N_2), presenting a refractive index sensitivity to bulk RI changes of 425 nm/RIU, which is very significant taking into account what is reported in literature. Furthermore, a 2-fold signal increase was observed for both O_2 and CO gases, showing that the thin film system is clearly more sensitive to these non-inert gases, due to, most probably, chemisorption. The results showed that the Au:CuO thin film system is a RI sensitive platform able to detect inert gases, which can be more sensitive to detect non-inert gases as O_2 or even other reactive gases as CO.



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Influence of a plasma treatment on the microstructure and plasmonic behaviour of Au-Al_2O_3 thin films

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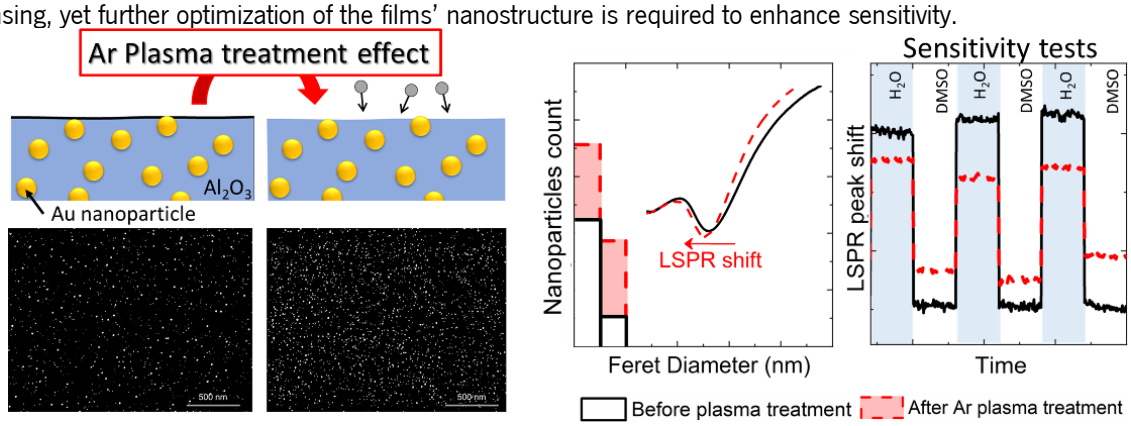
Keywords: Au-Al_2O_3 Thin Films, Sputtering, Localized Surface Plasmon Resonance

Abstract: Nanocomposite thin films, composed of noble nanoparticles dispersed in a dielectric matrix, have been considerably object of study since they exhibit peculiar properties due to the Localized Surface Plasmon Resonance (LSPR) phenomenon. The LSPR effect is based on the excitation of localized surface plasmons in metal nanoparticles' surface. The main goal of this work was to produce a sensitive and robust optical platform based on nanoplasmonic thin films composed of gold nanoparticles (Au) embedded in an Al_2O_3 matrix [1,2]. The Au-Al_2O_3 thin films were deposited by reactive DC magnetron sputtering and submitted to thermal treatments in order to promote the formation of Au nanoparticles. The Au concentration of the thin films varied from 8.9 at.% to 20.7 at.%. The increased annealing temperature on an optimized film caused a progressive crystallization of the Au nanoparticles, however the Al_2O_3 matrix remained roughly stoichiometric and amorphous. Nonetheless, the amorphous matrix limited the growth of Au nanoparticles up to 20 nm. Moreover, the application of an argon plasma treatment enabled the removal of superficial layers and allowed the increase of the density of Au nanoparticles partially exposed at the films' surface. The plasma treatment caused a blue-shift on the T-LSPR band since more nanoparticles are partially exposed. The plasma treatment also affected the refractive index sensitivity (RIS), which was found to be negative [1]. The plasmonic properties of this type of films can be used as a platform for plasmonic sensing, yet further optimization of the films' nanostructure is required to enhance sensitivity.



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Acknowledgements: This work was supported by the FCT in the framework of the Strategic Funding UID/FIS/04650/2019 and project NANO4BIO POCI-01-0145-FEDER-032299, with FCT reference PTDC/FIS-MAC/32299/2017. Diana I. Meira acknowledges FCT for her PhD Scholarship, SFRH/BD/143262/2019.

Influence of nanoparticle size and composition on the plasmonic response of Au-TiO_2 and Ag/Au-TiO_2 thin films

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Keywords: Localized Surface Plasmon Resonance, optical (bio)ensing, thin films, reactive DC magnetron sputtering, Transmission Electronic Microscopy.

Abstract: Plasmonic nanoparticles, such as Au and Ag, have been studied with the purpose of developing highly reliable, sensitive and label-free optical (bio)sensors. Characteristics of these nanoparticles, like size, distribution, shape and composition, can greatly affect the absorption band that arises from Localized Surface Plasmon Resonances. This effect is also found in magnetron sputtered thin films, composed by noble metal nanoparticles embedded in dielectric matrixes, and it is possible to change the optical properties of the of LSPR band of these thin films using post-deposition annealing. This thermal treatment induces changes in the morphology and crystallinity of both the matrix and the noble metal, promoting the formation of nanoparticles and altering their shape, size and distribution. This temperature dependent changes can be used to tune the LSPR band for its application in optical sensing, where shifts in the position of the plasmonic band can be used to detect the presence of molecules. In this work, different sets of thin films were produced by reactive DC magnetron sputtering to study the effect nanoparticle size and composition in the LSPR peak. To study the size distribution of the embedded nanoparticles, transmission electronic microscopy was used. Optical transmittance spectra were also measured, and refractive index sensitivities were calculated by measuring the optical response of the thin films to different media. The results showed that bimetallic Au-Ag nanoparticles can be used as the plasmonic material instead of pure Au nanoparticles, maintaining the same performance, with an obvious decrease of production costs.

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Acknowledgements: This work was supported by FCT in the framework of the Strategic Funding UID/FIS/04650/2019; and by the projects NANOSENSING POCI-01-0145-FEDER-016902, with FCT reference PTDC/FIS-NAN/1154/2014; project NANO4BIO POCI-01-0145-FEDER-032299, with FCT reference PTDC/FIS-MAC/32299/2017, and Transnational cooperation Portugal/France (Acordo Pessoa 2019/20). Diogo Costa and Marco S. Rodrigues acknowledge FCT for PhD Scholarships, SFRH/BD/136279/2018 and SFRH/BD/118684/2016.

Transparent Niobium-doped Titanium Dioxide Thin Films with high Seebeck coefficient for thermoelectric applications

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Keywords: thermoelectric materials, thin films, transparent conductive oxides, titanium dioxide

Abstract: Transparent conducting oxide (TCO) materials with thermoelectric properties is a promising technology to produce electrical energy through the harvesting of heat from the environment. As an alternative to the conventionally used TCO, ITO [1], TiO_2 has been extensively investigated due to its interesting optical and electronic properties and good stability in the adverse environment and a cationic doping of TiO_2 has been documented to improve its electrical conductivity [2]. In this project, TiO_2 (titanium dioxide) thin films doped with Nb (Niobium) were produced by reactive d.c. magnetron sputtering in high vacuum. These films are transparent in the visible region and show promising thermoelectric properties. The goal is to achieve both a high Figure of Merit and Power Factor, by increasing the electrical conductivity, decreasing the thermal conductivity and increasing the Seebeck coefficient of the thin films. Several process parameters were adjusted, such as reactive gas (O_2) partial pressure and deposition time and temperature, which affect the morphology and crystalline structure of the thin films [3]. Hence, by tuning these parameters and modifying the thin film's optical, electric, thermal and thermoelectric properties enables their suitability for application in photovoltaic systems, touch displays, amongst other devices, in order to render these more sustainable. Results so far show average transmittance in the visible region of up to 85 %, Seebeck Coefficient values of ~-200 $\mu V \cdot K^{-1}$, electrical resistivity of ~10^{-2} $\Omega \cdot cm$ and thermal conductivity of ~2 $W \cdot m^{-1} \cdot K^{-1}$. These results correspond to a PF of ~10^{-4} $\mu W \cdot K^{-2} \cdot m^{-1}$ and ZT of 0.1.

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Thermoelectric study of ZnO-based thin films: the effect of Bi dopant content.

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Keywords: Energy, Thin Film, Thermoelectric, Transparent, Zinc Oxide.

Abstract: This work reports on the optimization of the thermoelectric properties of ZnO-based thin films for applications that envisage coatings as transparent thermoelectric electrodes in devices [1]. As several reports indicate, point defects are very effective in controlling the thermal conductivity on oxide-based thermoelectrics [2]. The approach consists in introducing Bi ions, a higher mass element, into the ZnO metal-oxide matrix, in order to hinder phonon mediated heat conduction, whilst maintaining the Seebeck coefficient and high electrical conductivity. Hence, in this work, the effect of Bi dopants on ZnO-based thin films was investigated for three distinct Bi concentrations, two thickness (500 nm and 250 nm) and for three types of films: ZnO; ZnO:Al and ZnO:Ga, all produced by a custom-built d.c. magnetron sputtering setup in confocal geometry. The films were characterized concerning their: structural properties by X-ray diffraction and atomic probe tomography in order to verify the existence of secondary phases or Bi atoms segregation at the grain boundaries. Transport properties, namely resistivity, carrier concentration and mobility, were determined using a Hall effect equipment and compared to the same properties obtained by fits on optical properties, transmittance and reflectance measurements, in order to understand the Bi doping effect, on optically active carriers to study the role of grain boundaries. Furthermore, the thermal conductivity was assessed by frequency domain thermoreflectance and the Seebeck coefficient determined using a custom-made equipment. In the best-case scenario, a thermoelectric figure of merit of ≈0.01 was attained at room temperature.

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Water-based $CuIn_xGa_{1-x}Se_2$ chalcopyrite nanoink for flexible solar cells

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Keywords: photovoltaics, CIGSe, screen printing;

Abstract: Strong efforts are being carried out looking for efficient, clean and renewable energy sources to fulfill the ever-growing energy consumption. With respect to solar energy, inorganic thin film solar cells based on $CuIn_xGa_{1-x}Se_2$ (CIGSe) acquired special attention. The highest solar cell efficiency achieved with CIGSe as photo-absorber layer is, up to date 23.4%, prepared using vacuum-based deposition techniques. The use of non-vacuum deposition techniques is desirable due to the lower-cost of the process, scalability, and compatibility with flexible substrates. Solution-processed CIGSe thin film solar cells with an efficiency of 15.2% have been achieved, however a highly toxic procedure is used. A water-based and screen printable CIGSe photo-absorber layer for solar cells has been developed in the present work. This layer was achieved by dispersing different concentrations (23, 43 and 64wt%) of indium, gallium and copper oxides in water, using an ultrasound bath. The dispersion of the oxides was improved using different surfactants and the viscosity of the solution was adjusted with the addition of a hydrophilic polymer. An automatic screen printer was used to deposit the nanoinks over stainless steel. Finally, a thermal treatment (550°C for 30min) has been performed placing the samples inside a graphite box with Se pellets, to produce the final CIGSe crystals. The developed CIGSe water-based nanoinks present a colloidal behaviour and a tailorable viscosity compatible with screen printing technique. CIGSe phase-purity crystallinity was evaluated by XRD and Raman revealing the characteristic peaks of chalcopyrite, free of impurities. Morphological characterization revealed a dense CIGSe layer with few micrometers of thickness.

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Water-based graphene inks for printed electronics

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Keywords: Printed electronics; Screen-printing; Graphene; Thermo-resistive sensors

Abstract:
Printed electronics appeared as a promising alternative to conventional photolithography technology. Screen-printing process shows potential for mass production of large-area electronics at very low cost, allowing patterning, and it is a simple, scalable and environment-friendly process.
Conductive screen-printing inks generally contain three components: conductive nano- or microparticles (as filler), organic binder/additive, and solvent. Graphene has attracted significant interest for a wide variety of applications due to its outstanding mechanical, thermal, and electrical properties, making him an excellent candidate for printed flexible electronics. Remarkable electronic properties as electrical conductivity combined with specific surface area made graphene in widely used material for piezo-resistive [1] and thermo-resistive [2] sensors. Carboxymethyl cellulose (CMC) used in the form of its sodium salt, is a hydrophilic cellulose derivative that can be used to help suspend graphene in the preparation of the inks [3]. To concretize the ambitious goal of eco-sustainability, one solution is the development of water-based inks, replacing organic based solvents.
Conductive graphene inks using CMC as a functional polymer were developed, and $\sigma = 1.8\text{x}10^{2}\ \Omega.\text{m}$ was obtained. We combine the best electrical properties of the graphene with chemical and mechanical properties of the CMC as binder to develop novel functional inks for screen-printing process to produce conductive inks, piezo-resistive and thermo-resistive sensors (-34.65 Ω/°C ± 0.55 Ω/°C).

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Mechano-electrical skeletal muscle cell stimulation for tissue regeneration

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Keywords: magnetoelectric biomaterials, skeletal muscle tissue engineering, mechano-electrical stimuli, myotubes.

Abstract: The prevalence of skeletal muscle disorders has been steadily increasing worldwide, requiring new strategies for their structural and functional regeneration. Piezoelectric polymers have attracted interest offering new opportunities for skeletal muscle tissue engineering (TE), since they are electromechanically active, allowing tissue mechano-electric and electro-mechanical stimulation [1]. Physical stimuli have demonstrated to be important parameters to be considered for tissue engineering, but poorly applied in muscle regeneration. In this context, this work reports on magnetoelectric biomaterials suitable for effective proliferation and differentiation of myoblast in a biomimetic microenvironment providing the electro-mechanical stimuli associated to this tissue in the human body. Magnetoelectric films are obtained by solvent casting through the combination of a piezoelectric polymer, poly(vinylidene fluoride-trifluoro-ethylene), and magnetostrictive particles ($CoFe_2O_4$). The non-poled and poled (with negative and positive surface charge) magnetoelectric composites were used to investigate their effect on C2C12 myoblast adhesion, proliferation and differentiation. It is demonstrated that the proliferation and differentiation of the cells was enhanced by the application of mechanical and/or electrical stimulation comparatively to the static conditions, with higher values of maturation index under mechano-electrical stimuli combined with chemical stimuli (differentiation medium) up to ≈ 70%. Further, direct mechanoelectric dynamic stimulation also increases the maturation index of myotubes. These results showed that mechano-electrical cell stimulation is a novel and full potential approach for skeletal muscle tissue engineering applications.

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High magnetoelectric response materials for all-printed electronics

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Keywords: Magnetoelectric, Sensors, Printed Electronics.

Abstract: Two decades ago, the "polymer based magnetoelectric" idea changed thinking in magnetoelectric (ME) materials scientific community, which led to a new generation of powerful materials and an increased focus on controlling materials properties, as well as in the implementation into real applications[1]. Nowadays, the successful application of those materials is closely related to the processing and integration of ME materials by additive manufacturing techniques on the cutting edge interface of materials science with chemistry, physics, biology and engineering[2]. Here a novel screen-printed and flexible ME material is developed based on poly (vinylidene fluoride) – (PVDF-CFO) as the magnetostrictive phase. The all printed ME composite exhibits a ferromagnetic behavior with 16 emu g^{-1} saturation magnetization, -26 pC N^{-1} piezoelectric response and a ME voltage coefficient (α) of 164 mV cm^{-1} Oe^{-1} at a longitudinal resonance frequency of 16.2 kHz. Such optimized magnetic, piezoelectric and ME behavior associated with the reduced cost of assembly and large areas trough screen printing demonstrates the suitability of the developed material for applications such as printed electronics, sensors, actuators and energy harvesters.

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Evaluation of the bacterial response to piezoelectric microenvironments

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Keywords: piezoelectric material, bacteria, anti-/pro-microbial, mechanoelectric effect, surface charge

Abstract: Taking advantage on the ability of bacteria to adapt to different environments, this work investigates the effect of electrically active microenvironments on these microorganisms. Electrical microenvironments were developed via mechanical stimulation of a piezoelectric polymer, generating an electrical response [1]. Gram-positive *Staphylococcus epidermidis* and Gram-negative *Escherichia coli* were grown on the surface of piezoelectric poly(vinylidene) fluoride (PVDF) films to study bacteria behaviour under: (i) the effect of the material surface charge in static conditions, (ii) the mechanical effect, and (iii) the piezoelectric effect, the last two achieved under dynamic conditions. Bacteria viability in planktonic and biofilm forms were measured, and their morphology was characterized. Whereas *E. coli* responds little to any of the stimuli application, *S. epidermidis* growth can be regulated through the material surface charge and by the applied frequency. Positively charged PVDF induces bacterial growth inhibition in planktonic and adhered cells in static conditions, whereas antifouling properties are obtained when a mechanical or piezoelectric effect at 4 Hz stimuli is applied. However, by increasing the stimuli to 40 Hz, the bacteria adhesion is promoted [2]. In conclusion, the behaviour of certain bacteria species is tailored through the application of piezoelectric materials, allowing the design of suitable anti- and pro-microbial strategies. These strategies are only found in mammalian cells studies, whereas in bacterial cells such stimulation is still unknown. Thus, this work provides one of the first insights on the effect of the piezoelectric stimuli on bacterial cells.

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Thermochromic and Thermoresistive Ionic Liquids based Printable Materials

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Keywords: electroactive materials, ionic liquids, PVDF, smart materials, thermochromic

Abstract: Thermochromic materials have been gaining increasing attention due to their ability to reversibly change color as a function of temperature. Those materials can be applied in several areas, including energy, flexible electronics, textile industry, and smart food packaging, among others. Combining ionic liquids (ILs) with a polymeric matrix offers many advantages when compared to traditional materials, based on the high versatility and high-potential building blocks, allowing to combine the characteristics of the ILs with the key features of polymers[1].
In this work, reversible thermochromic and thermoresistive materials based on PVDF and the IL $[Bmim]_2[NiCl_4]$, with different IL contents (10,20 and 40 % wt.) were prepared using the solvent casting method. The thermochromism, physicochemical, electrical, and thermal properties were evaluated at different temperatures. UV–vis and X-ray analyses revealed that a reversible thermochromism behavior (transparent to blue or vice-versa). An increase in the electroactive β-phase content and crystallinity of PVDF is obtained with the presence of the IL. Electrical measurements show an increase in the electrical conductivity with both increasing $[Bmim]_2[NiCl_4]$ content and temperature[2].The developed materials shows a large potential for the development of thermochromic and thermoresistive printable sensors in areas such as temperature and water level sensors and smart windows, among others.

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Development of magnetoelectric materials for printed electronics

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Keywords: magnetoelectric, energy harvester, sensor, transparent

Abstract: The "Internet of Things" concept is triggering one of the biggest technologic revolutions, with impact in different areas, such as industry, energy and environment.
The present work reports on the fabrication, characterization and incorporation of smart and multifunctional magnetostrictive and magnetoelectric printed materials, in energy harvesting and magnetic sensor applications (1). The fabrication and functional characterization of magnetostritive ink based on poly(vinylidene fluoride), PVDF, and CoFe2O4, magnetoelectric ink based on PVDF+CoFe2O4/PVDF-TrFE) (2), as well as optically transparent (3) magnetoelectric materials allows the development of magnetoelectric energy harvester and sensor, respectively.
The development of the inks, the characterization of the printed layers and the performance of some representative devices will be presented and discussed.

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Micropatterned electroactive polymers for biomedical and energy applications

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Keywords: poly(vinylidene fluoride- co-trifluoroethylene), membranes, microstructures, cell adhesion, separator.

Abstract: Micropatterned piezoelectric poly (vinylidene fluoride-co-trifluoroethylene) – P(VDF-TrFE) membranes were tailored with dense and porous morphologies. Surface patterns (lines, intermittent lines, hexagons, linear zigzags, curved zigzags and pillars, with dimensions of 25, 75 and 150 μm) were processed resorting to polydimethylsiloxane–(PDMS) molds fabricated by soft lithography. For TE applications, the micropatterned membranes were tested as scaffolds in cell adhesion assays of myoblasts and pre-osteoblasts cell lines. The results shown that cell adhesion site, orientation and elongation can be controlled by the physical stimuli given with the topography and morphology of the scaffolds. Linear surface topographies with dense morphology presented a large potential in the regeneration of musculoskeletal tissue, while more anisotropic surface microstructures with porous morphology in the growth and regeneration of bone tissue [1]. Regarding energy applications, patterned membranes with 75 μm and porous morphology were tested as battery separators. It was shown that micropatterning significantly improves battery performance, with the zigzag micropatterned separator promoting a discharge capacity efficiency of batteries in an 804% higher than the ones with non-patterned separators [2]. This work proves the value of these tailored membranes in two very different areas.

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Ionic-Liquid-Based Electroactive Polymer Composites for Muscle Tissue Engineering

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Keywords: electroactive, ionic liquid, PVDF, smart materials, tissue engineering

Abstract: As an electromechanically active tissue, muscle regeneration takes advantage of scaffolds that are able to mimic the natural microenvironment of muscle cells through mechanoelectrical stimuli. This works reports on ionic electroactive materials based on poly(vinilidene fluoride) (PVDF) and ionic liquids (ILs) for muscle tissue engineering. IL/PVDF composites comprising different IL contents of 1-butyl-3-methylimidazolium chloride [Bmim][Cl] and 2-hydroxyethyl-trimethylammonium dihydrogen phosphate [Ch][DHP] were obtained by solvent casting. The morphological, physico-chemical, thermal and mechanical properties of the composites was evaluated, as well as their citotoxicity. Besides of improving the electrical conductivity, the incorporation of [Bmim][Cl] and [Ch][DHP] promotes the PVDF crystallization into the polar β-phase and also influences the thermal stability of the composites. Moreover, the incorporation of both ILs leads to a strong reduction of the elastic modulus, indicating that ILs act as a PVDF plasticizer whitin the polymeric matrix. Finally, the noncytotoxicity of the IL/PVDF composite films and C2C12 cell proliferation demonstrates the applicability of the composites as a suitable platform for active muscle regeneration strategies [1,2].

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Nano and micro materials for highly efficient arsenic removal from water

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Keywords: Adsorption, arsenic, heavy-metals, nanomaterials, water remediation

Abstract: Water pollution is a growing problem, mainly caused by uncontrolled water contamination. In this scope, one of the major environmental concerns is the presence of heavy metals in water. Arsenic (As) is one of the twenty most abundant elements in the environment, and it is considered one of the most potential carcinogens [1]. Long term arsenic exposure causes skin lesions, cancer, cardiovascular diseases, pulmonary problems, neurological deficiencies and developmental and reproductive toxicity [2]. The application of nanomaterials for the removal of As from contaminated water represents one of the most promising remediation approaches nowadays [3].
In this study, three active materials, including yttrium carbonate, hematite and 10 wt. % ZnO/TiO_2, have been prepared and characterised, and their arsenic adsorption capacity in water evaluated. Thus, the adsorption behaviour, including the isotherms, kinetics, the influence of pH, time of contact and initial concentration of As in solution were evaluated.
This work demonstrates that ZnO/TiO_2 nanocomposite shows a high adsorption performance, with adsorption efficiencies always close to 100%, leading to a maximum adsorption capacity of 42.27 mg/g. These remarkable adsorption results indicate the suitability of 10 wt.% ZnO/TiO_2 nanocomposite for application in arsenic removal from contaminated water.

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Surface engineering of nanostructured Ta surface with incorporation of osteoconductive elements by anodization

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Keywords: Tantalum; Anodization; Biofunctionalization; Calcium Phosphates; Magnesium

Abstract: Surface modifications have been deeply investigated to improve their properties (nano-morphology/topography and chemistry), mainly to enhance surface bioactivity and consequently to overcome the current dental implants failures. For this purpose, the main goal of this work is to mimic the bone morphology as well as its chemical composition by the incorporation of calcium (Ca), phosphorus (P) and magnesium (Mg) on a tantalum (Ta) surface. Two approaches were used: reverse polarization (RP) and/or anodization, under different applied potential and acid-free electrolytes. It was observed that RP followed by anodization promoted the incorporation of cations (Ca^{2+}, Mg^{2+} and Na^{+}) in a competitive way. X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) analyses showed formation of amorphous calcium phosphate compounds. Moreover, a surface enriched with Ca, P and Mg achieved a Ca/P ratio of 1.4 similar to the stochiometric hydroxyapatite (1.67). The surfaces subsequently became rougher and hydrophilic with their biofunctionalization. All these surface features are good pointers towards a better implant osseointegration.

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Alternative coatings to hexavalent chromium in applications under cyclic loads

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Keywords: sputtering, minting, hexavalent chromium, hardness, nano-impact

Abstract Aiming to improve the protection of human health and the environment, REACH regulation was enforced across EU, accelerating the need to find a viable alternative to industrial electrodeposition processes. Electroplating parts with hard chromium is associated to professional diseases and environmental concerns also play a role in this, because hexavalent chromium is a pollutant related to water and soil contamination. Electroplated chromium coatings are widely used due to its physical properties that allow a longer service life of products that usually fail because of wear. Minting is one of those application where the good mechanical and tribological properties of hard chromium were never outmatched by any other coating.

Our goal is to prepare a tool material which has all the required properties comparable to hard chromium. In our work CrN, CrAlN and CrAlSiN coatings were produced by reactive DC magnetron sputtering technique. Two different interlayer configurations were used, and samples were deposited either with a single Cr adhesion interlayer or several layers with increasing N content.

Focusing on mechanical properties, an increase in hardness was observed with consecutive addition of elements in CrN matrix as expected, ranging from aprox. 10 GPa in CrN coatings to aprox. 30 GPa in CrAlSiN coatings.

After nano-impact tests we observed that CrAlN coating had the best performance and no crack events by fatigue were observed in SEM after 50 impacts. According to H/Er ratio and plasticity index, CrAlN and single adhesion layer CrN samples can be considered very good candidates for cyclic loads applications.

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Multifunctional coatings based on doped Ag-TiN for 3D printed ceramic pieces

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Keywords: Additive manufacturing, Multifunctional, Titanium nitride, Antibacterial, Antibiofouling.

Abstract: Additive manufacturing (AM) is a hot topic nowadays, having a first order in importance in research trends, improving existent technologies and carrying them further. AM can be applied to ceramics, which have importance in current technologies. Their capability to maintain functional properties for long time periods, combined with the easiness to process and the abundance of raw materials, make them a fundamental part of mankind development. Within ceramics, stoneware has a wide range of uses but in some conditions, it can be affected by biofouling. Ti(O)N and Ag-Ti(O)N coatings over 3D printed stoneware, were presented as multifunctional solution, linking aesthetical and antimicrobial properties. Films were developed by reactive direct current (DC) magnetron sputtering and characterized physical, chemical and morphologically, as well as regarding their color variation. Moreover roughness, wettability, antibacterial and antibiofouling were also evaluated. The results revealed that the Ag doped coatings (with or without oxygen addition) had an enhanced multifunctionality compared to control samples (without Ag). Ag nanoparticles addition created a surface with antibacterial and antibiofouling, in order to resist outdoors and aqueous environments, making these films able to be applied in architectural pieces as sculptures or other decorative parts, maintaining their properties with good aesthetical properties.

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TiSiN(Ag) coatings deposited by HiPIMS

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Keywords: HiPIMS, Structure, Annealing, Oxidation, Tribology

Abstract:
TiSiN(Ag) coatings with Ag contents ranging from 0 to 29 at.% were designed as promising materials to allow long term solid lubrication during dry machining operations. Introduction of silver pellets on the target progressively increases the Ag concentration on the films, influencing the deposition rate, structure and morphology of the films. Hardness and Young's modulus of the coatings decreased with increasing Ag additions mainly due to the increase of this soft phase on the microstructure. Annealing treatment didn't present any significant changes in the structure/phase composition or mechanical properties of the coatings. Silver diffusion appears to be controlled after the annealing treatment. Dynamic-mode thermogravimetry analysis showed that silver addition does not change the onset point of oxidation of the coatings. However, the oxidation rate deteriorated with the presence of Ag. An unusual mass loss could be observed for the coatings with 6 and 10 at.% of Ag, as a result of silver evaporation/sublimation process. Results from isothermal thermogravimetry performed at 900 °C show two distinct regimes and corroborate the detrimental effect of the Ag on the oxidation resistance of the coatings. Nonetheless, in the un-oxidized part of the films, the silver continued to be homogeneously distributed confirming again the efficient barrier against Ag diffusion. Tribology tests showed that by increasing the silver content in the films, the COF is slightly reduced. Most importantly, when the test temperature was increased to 900°C, the amount of adhered material was clearly reduced with the increase in the Ag content.

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Oxidation of Metallic and Bimetallic Nanoparticles Produced by Magnetron Sputtering

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Keywords: Zinc-Iron, sputtering magnetron, nanoparticles, oxidation

Abstract: In recent years, nanomaterials have gained a huge intention in scientific investigations, due to their ability of surface modification and multifunctionality. Many previous studies focused on applying metallic nanoparticles for industrial applications, which depending on their nature can act as antibacterial agents, antioxidants, and catalysers, among others [1-3]. In addition, bimetallic nanoparticles have shown enhanced functional characteristics since such nanostructures exhibit not only the properties of their constituents, but also synergetic new phenomenology due to physical binding between their components. As a result, in the present research, metallic and bimetallic NPs were produced by magnetron sputtering, in order to study their oxidation process by the change of their colors. Zinc and Iron NPs were produced in two different methodologies, one with the classical magnetron sputtering, and the other with a hybrid system composed by cluster gun and magnetron sputtering. All depositions were performed in Ar atmosphere varying the current density, from 0.1 to 0.5 A, and deposition time. The morphology and elemental analysis were characterized by scanning (transmission) electron microscopy (SEM and STEM), energy dispersive spectroscopy (EDS) and selected area electron diffraction (SAED). The images were acquired using a FEI Titan ChemiStem operated at 200 keV, while the color measured were carried out in a CM-2600d/MINOLTA spectrometer. The results demonstrate various distributions, sizes, Zn/Fe fractions and colors of the films, which can be partially controlled by the deposition parameters and the environment in which they are stored.

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Effect of morphology on the wear behaviour of CrN coating deposited by arc-PVD method

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Keywords: piston ring, coating, morphology, tribological performance

Abstract: PVD films are widely used in automotive industry for tribological purposes. In heavy-duty diesel engines, piston rings represent a challenging component concerning its tribological performance. Top piston rings were designed as an additional part with a supporting role in the sealing or prevention of gas leakages from the combustion chamber. Several works have been published proposing metal nitride coatings for the piston ring functional surface. CrN coatings are among those most frequently proposed, but regularly using magnetron sputtering as the predefined deposition method. In a large-scale production framework different deposition method with improved deposition rates must be adopted. Cathodic arc deposition is currently widely implemented in several industries, such as automotive. Although this technique is consolidated in the industrial environment, the deposition process and parameters are continuously under optimisation. Even using the same targets, the final properties of the deposited coating are strongly dependent on the chamber conditions.
In the present work are studied two different CrN coatings deposited in the piston ring functional surface. Using different deposition conditions two distinct morphologies are achieved in the coating layer: a more sense structure (CrN-A) and a columnar structure (CrN-B). Those coatings were tested using a locally developed test rig, adapted to test the piston rings under conditions close of the real engine operation. The surface was characterised using SEM and EDS techniques before and after to perform the wear and friction tests.

Acknowledgements: This work was supported by FCT (Fundação para a Ciência e Tecnologia) and MAHLE, Componentes de Motores, S.A under Grant SFRH/BDE/110654/2015.

A Polynomial Approach to the Spectrum of Dirac-Weyl Graphene Flakes

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Keywords: Graphene, Dirac-Wyel, Flake, Polynomial, Boundary Conditions

Abstract: The initial objective of this work was to study the angle dependence of the spectrum for the regions of dominant AA-stacking in twisted bilayer graphene using a continuum method[1]. These regions are hexagonal, which means that we must first find a way to solve the Dirac-Weyl equation in polygonal enclosures.
Due to the inexistence of analytical solutions of partial differential equations for most polygonal enclosures, we replicate a method used originally in the study of flexural vibrations of regular polygonal plates[2].
With this method, we obtain the low-energy eigensystem of Schrödinger's equation, in polygons with hard boudaries, which we compare to existing exact theoretical results, and to numerical diagonalization of the Laplacian operator.
To address the spectrum of the Dirac-Weyl equation in finite regions, we first review possible types of boundary conditions[4] and generalize the polynomial method for two component spinors.
We were able to replicate an exact solution for a triangular flake with boundary conditions such as found in graphene zig-zag edges[3,5]. We found, however that this is a very special case, essentially equivalent to the solution of Schrödinger's equation.
We also sudied hexagonal and square shaped flakes, with more general boundary conditons, which constitute a non-trivial generalization of the polynomial method for two component spinors.

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Edge-magnetism in Transition-metal Dichalcogenide Nanoribbons

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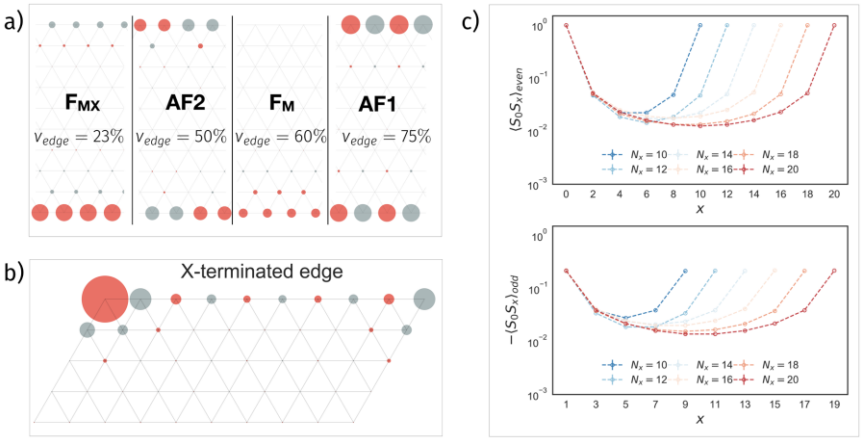
Keywords: Edge-magnetism, Transition-metal dichalcogenide nanoribbons, Mean Field Theory, Determinant Quantum Monte Carlo

Abstract: Transition-metal dichalcogenides (TMDs) are 2D materials with ample prospective technological application. In particular, TMD nanoribbons (TMDNRs) may host edge-magnetic phases emerging from electron-electron interactions, similarly to graphene. Thus, they could be used in spintronics, provided that the electronic spin can be manipulated, for example by a back gate voltage or a magnetic field. We probe edge-magnetism in zigzag-terminated TMDNRs. We consider a 3-band tight-binding model with an added intra-orbital Hubbard term. We use Mean Field Theory (MFT) and determinant Quantum Monte Carlo (detQMC), comparing the results obtained with each method. Mean Field Theory predicts two gapped phases at the chalcogen (X) and transition-metal (M) terminated edges for specific edge fillings, namely a dimer and an antiferromagnetic phase. Away from the gapped phases, MFT indicates that a ferromagnetic phase sets in. detQMC results confirm the stability of this antiferromagnetic phase.



a)MFT magnetic ordering for Hubbard interaction U = 2.94 eV at temperature T = 0 K. The size of the circles indicates the magnitude of the spins. Red corresponds to spin-up and blue to spin-down. b) Spin-spin correlations with respect to the leftmost site of the X-edge, measured with detQMC for a 10x5 molybdenum disulfide nanoribbon with U = 2.94 eV and T = 267 K at three-quarter edge filling.

. Red corresponds to a positive correlation and blue to a negative correlation. c) Spin-spin correlations on the X-edge for the same parameters of b), for varying longitudinal length N_x of the ribbon.

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Acknowledgements: The authors acknowledge financing from Fundação da Ciência e Tecnologia and COMPETE 2020 program in FEDER component (European Union), through the projects POCI-01-0145-FEDER-028887 and UID/FIS/04650/2013.

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RP02	**Applications of real-time measurement of ocular aberrations** Jessica Gomes and Sandra Franco
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RP12	**Electroactive polymer-based microstructures for biomedical applications** André S. Macedo, E.S. Pimentel, V.F. Cardoso, D.M. Correia, G. Botelho, S. Lanceros-Méndez
RP13	**Antifungal action of ZnO thin films prepared by glancing angle deposition** Patrícia Pereira-Silva, Augusto Costa-Barbosa, Diogo Costa, Marco S. Rodrigues, Paula Sampaio, Joel Borges, Filipe Vaz
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RP15	**Enhanced ionic conductivity in electrospun separator membranes based on poly(vinylidene fluoride) blended with different ionic liquids for lithium-ion battery applications** João C. Barbosa, D. Correia, R. Gonçalves, C. M. Costa, V. de Zea Bermudez, M.M. Silva and S. Lanceros-Mendez
RP16	**Analytical expressions for the second order conductivity of a cold semiconductor** Gonçalo B. Ventura, D. J. Passos, J. M. V. Parente Lopes, J. M. B. Lopes dos Santos
RP17	**Magnetic dipolar synchronization of vortex-based spin torque nano-oscillators with independent top contacts** Leandro Martins, Alex Jenkins, Jérôme Borme, João Ventura, Ricardo Ferreira and Paulo Freitas
RP18	**(Para)magnetic nanocarriers for early detection and treatment of solid tumors** Cátia Rocha, Manuel Bañobre-López, Juan Gallo
RP19	**Fluorescent Effect on Textile Supercapacitors** Joana S. Teixeira, André M. Pereira, Clara Pereira
RP20	**Orbital Hall effect in Transition Metal Dichalcogenides monolayers** Tatiana G. Rappoport
RP21	**Self-assembling of dipeptide nanotubes inside electrospun fibers with strong piezoelectric response** Rosa M. F. Baptista, Etelvina de Matos Gomes, M. Manuela M. Raposo, Susana P.G. Costa, Paulo E. Lopes, Bernardo Almeida, Michael S. Belsley
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RP25	**Environmental remediation strategies based on polymernanocomposites** Pedro M. Martins, H. Salazar, J.Teixeira, and S. Lanceros-Mendez
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Ocular biometry and refractive error of a Young Portuguese Subjects during 3 years of University Enrolment

Daniela Lopes-Ferreira*, Ana Rita Oliveira Vaz, Rute J. Macedo-de-Araújo, Ana Amorim-de-Sousa, Paulo Fernandes, Ana F. Mota, André Amorim, Miguel Faria-Ribeiro, Sofia Peixoto-de-Matos Antonio Miranda, Jorge Jorge, António Queirós, José Manuel González-Méijome

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Keywords: myopia, refractive error, corneal radius.

Abstract: **Purpose:** To evaluate the ocular corneal curvature, axial length and refractive error in young Portuguese students by gender and age in 3 consecutive years, during the university enrollment. **Methods:** Subjects aged among 17 to 25 years were evaluated in 2016, 2017 and 2018 during their 1st university enrollment at University of Minho, Braga, Portugal. Corneal curvature, axial length and non-cycloplegic refractive error were measured by IOLMaster Optical Biometer and by Grand Seiko WAM-5500 Open-Field Autorefractor, respectively. **Results** A total of 821, 835 and 773 subjects were evaluated at 2016, 2017 and 2018, respectively. Mean age of subjects was 18.82±1.26, 18.61±1.00, 18.54±1.00 years ($p<0.05$), being 39%, 36% and 33% male, respectively in 2016, 2017 and 2018. Comparing subjects by age, no statistical differences were found to neither variable, in any of the year. Exception to subjects with age 18 that presented Kflat of RE (mean diff 0.16±0.04mm, $p=0.001$) and LE (0.14±0.04mm, $p=0.012$) flatter than subjects with 20, in 2017. In 2016, males were slightly older ($p=0.047$), presenting REs longer (0.44mm) and Kflat of RE and LEs flatter (mean diff 0.13mm and 0.12mm) than female. Similarly, in 2017 and 2018, male presented both eyes longer (0.51mm, 0.51mm // 0.58mm, 0.59mm, $p<0.001$) and Kflat of both eyes flatter (0.14mm, 0.13mm // 0.14mm, 0.14mm, $p<0.001$). At 2018 male also presented greater myopia at LE (mean diff 0.15D, $p=0.03$). **Conclusions:** Male subjects evaluated manifested a tendency to present longer eyes and flatter corneas, and in some cases greater degree of myopia than females.

Applications of real-time measurement of ocular aberrations

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Keywords: Aberrometry; Accommodation; Ocular Aberrations

Abstract: Aberrometry is one of the techniques available for the measurement of the optical quality of the eye. It has been applied clinically and shown to be an important evaluation tool.
Here a new methodology to assess how the aberrations change with the accommodative eye is presented. This methodology permits in-vivo and in real-time accommodative stimulation and simultaneous acquisition of the variations of ocular aberrations. A system with several negative lenses that stimulate the ocular accommodation, coupled with a wavefront sensor by using a Shark-Hartmann sensor, was developed. These two systems are synchronized, allowing the detection of the ocular aberrations while the eye is under the influence of the accommodative stimulus.
Algorithms to calculate some accommodative parameters were developed, thus enabling to obtain detailed information about the ocular accommodation behavior under different viewing conditions. Through these, it is possible obtain in real-time, the accommodative response and lag, its frequency, velocity, acceleration and the response time of the ocular accommodation and its relaxation.
This methodology was applied in real cases, focusing on the applications to symptomatic patients who do not present changes in the regular optometric exams in use in the optometric clinical practice, but are detected by applying this methodology.
Results showed that the real-time measurement of the ocular aberrations has several applications, for example for studying the variations of the optical proprieties of the eye to have a better and comprehensive knowledge of the eye and in helping in the clinical diagnosis of patients with accommodative dysfunctions and posterior follow-up.

Acknowledgements: This work was supported by the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2019 and by the project PTDC/FIS-OTI/31486/2017.

The influence of coloured lighting on accommodative parameters in subjects with accommodative dysfunctions

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Keywords: Accommodative amplitude; Accommodative flexibility; Illumination.

Abstract: The aim of this study was to assess if the color of the illumination influences the accommodative parameters in a population with accommodative dysfunction (AD). It was also assessed if there is a specific color that impacts the accommodation the most.
Seventeen subjects, aged 19 to 25 years (20.94±1.68 years), participated in the study. All subjects were previously diagnosed with AD by performing a complete optometric consultation. Using as illuminant the LED tunable lamp Ledgima luminary, the amplitude of accommodation (AA) and the accommodative flexibility (AF) were measured for three types of illumination: white, red and green.
The AA values obtained under the different lighting conditions were compared and it was found that there were statistically significant differences between the values determined under the white (8.79±1.97 D) and the red (7.63±2.05 D) illuminant, and the red and the green (8.34±2.67 D). The values obtained with the green and red illuminations showed no statistically significant differences. For the AF values, statistically significant differences were found between the values determined under the white (2.9±3.8 cpm) and the green (1.3±3.2 cpm), and the white and the red (1.2±2 cpm) illuminations. For the green and the red illuminations no significant statistical differences were found.
In conclusion, the AA is influenced by the color of the illumination, where the red illuminant presented the lowest values. On the other hand, the white illuminant presented higher values for AA and AF. The green and red illuminants showed statistically identical results for AF.

Acknowledgements: This work was supported by the Portuguese Foundation for Science and Technology (FCT) under the project PTDC/FIS-OTI/31486/2017.

The Influence of the Coloured Lighting on Amplitude of Accommodation

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Keywords: LED; Light; Colour; Ocular Accommodation

Abstract: The purpose of this work was to evaluate the influence of defined lighting parameters as illuminance, colour and colour temperature, on ocular accommodation. The amplitude of accommodation of 26 subjects, was measured and compared under normal lighting conditions (assuming white LED light) and under different illuminance levels (30lx, 150lx and 400lx), coloured lighting (green and red) and under different correlated colour temperature (2500K and 4500K). Measurements were done using a Ledigma luminary (Ledigma Ltd, Vilnius, Lithuania). Considering the illuminance, there was a statistically significant increase in the amplitude of accommodation from 30lx to 150lx ($p<0.001$). The amplitude of accommodation measured with 400lx illuminance also showed a statistically significant increase ($p<0.001$) when compared to that obtained with 30lx illuminance. However, the amplitude of accommodation measured with the illuminance of 150lx did not present statistically significant differences when compared to that obtained with the illuminance of 400lx ($p>0.05$). Regarding the coloured lighting, the accommodation amplitude values presented significantly lower values with red lighting when compared with those obtained with white light ($p=0.016$). Accommodation amplitude measured under red illumination, showed a statistically significant decrease when compared to that obtained with the green colour ($p<0.001$). However, the amplitude of accommodation measured with green light did not present statistically significant differences when compared to that obtained with white light ($p>0.05$). The same happened to the colour temperature, where no statistically significant values were found between 2500K and 4500K ($p>0.05$). Results seemed to show that particular light conditions influenced the amplitude of accommodation.

Acknowledgements: This work was supported by the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2019 and by the project PTDC/FIS-OTI/31486/2017 and POCI-01-0145-FEDER031486

The influence of coloured lighting on binocular vision

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Keywords: Binocular Vision; Fixation Disparity; Fusional Vergence; Illumination; Phoria.

Abstract: Light has influence at various points in our daily lives. We are increasingly exposed to various lighting conditions, both in our surroundings and during the use of digital devices. It is known that symptomatology is associated with tasks performed under inappropriate illumination conditions. Therefore, this study aims to evaluate the effect of color illumination on binocular vision.

The data collection consisted in two phases. First, a complete optometric examination was performed on 37 subjects, and they were selected only those who satisfied the inclusion criteria. Therefore, 24 subjects aged between 19 and 30 years old (22.3 ± 3.03 years old) were selected, where 79.2% were female. Phoria, positive and negative vergence and fixation disparities were then evaluated with different randomized lighting colors (white, green and red). Statistically significant changes were found only for the values of the phoria and fusional vergences. For the phoria it was found difference of 2 Δ between the green and white light ($p = 0.021$), and green and red colors ($p = 0.007$). For the fusional vergences changes were detected for the break and recovery values of negative fusional vergence and for the recovery of positive fusional vergence. The differences found for phoria can be explained by the longitudinal chromatic aberration, where the value of exophoria with green light was higher. The reproducibility of the method was attributed as the main factor for differences shown in the fusional vergence values. There were no significant differences detected for fixation disparity.

Energy storage characteristics of ferroelectric-dielectric multilayered thin films

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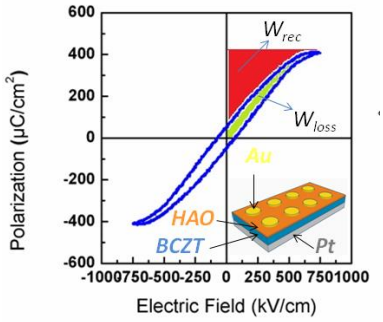
Keywords: energy storage performance, ferroelectric-dielectric structures, charge coupling effect.

Abstract: Among the various available electrical energy storage devices, such as batteries, supercapacitors and dielectric capacitors, the dielectric capacitors exhibit unique advantages such as ultrafast charge-discharge speed and high energy storage density.[1,2] Moreover, among them, the ferroelectric film capacitors usually possess short charge-discharge time (in the ns range), that make them suitable candidates for fast energy storage applications.[3] In the present work, the effect of the insertion of a thin dielectric HfO_2:$Al2O_3$ (HAO) layer at different positions in the Pt/0.5Ba($Zr0_{0.2}Ti0_{0.8}$)O_3-0.5($Ba_{0.7}Ca_{0.3}$)TiO_3 (BCZT)/Au layered structure on the energy storage performance of the capacitors has been investigated. The higher storage performance is achieved through the insertion of a HAO layer between the BCZT layer and the Au one. The insertion of the dielectric layer causes a depolarization field which results in a highly linear hysteresis loop with low energy dissipation. The Pt/BCZT/HAO/Au capacitors show an impressive energy storage density of 99.8 J/cm^3 and efficiency of 71.0%, at an applied electric field of 750 kV/cm. By combining ferroelectrics and dielectrics into one single structure, the proposed strategy provides an efficient way for developing high efficient energy storage capacitors.



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Tenofovir disoproxil fumarate/emtricitabine-loaded electrospun fibers for vaginal administration and prevention of HIV transmission

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Keywords: electrospun polymeric fibers, liposomes, drug delivery, microbicides

Abstract: The incidence of HIV is still a global concern. Women are highly vulnerable to sexual transmission so new prevention strategies are necessary. Microbicide products containing tenofovir disoproxil fumarate/emtricitabine (TDF/FTC), administered directly in the vagina for example in hydrogel form [1], could avoid early viral transmission at the mucosal level.
Hydrophobic fibers, of polycaprolactone (PCL), and hydrophilic ones composed by drug-loaded liposomes (DMPC:Chol:DOPE, 7:2:1) incorporated into poly(vinyl-alcohol) (PVA), were produced by electrospinning as potential vaginal delivery systems for TDF/FTC.
PCL and liposomes/PVA fibers were characterized by scanning electron microscopy and present mean diameters of 700 and 150 nm, respectively. Structural and mechanical properties were also assessed. Drug release in micellar medium at pH 4.5 was fast (within 15-30 min) and nearly complete for both fibers. Also, strong interaction with mucin, studied by fluorescence quenching, indicates that fibers (particularly PCL ones) may feature high vaginal retention. The toxicity of drug-loaded fibers to CaSki and HEC-1-A genital cell lines evaluated by MTT assay was negligible. *In vivo* experiments in mice showed that liposomes/PVA fibers were able to significantly enhance TDF and FTC concentrations, as compared to PCL fibers and oral Truvada® however, PCL fibers also presented higher drug levels in vaginal lavages than oral Truvada®. In all cases drug levels in lavages were undetectable 4 h after administration. TDF and FTC levels in vaginal tissues were near the detection limit, while systemic exposure was negligible for fibers.
Our results suggest that liposomes/PVA fibers may constitute an interesting microbicide system for vaginal delivery of TDF/FTC.

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Acknowledgements: Funding for this work was provided by Fundação para a Ciência e Tecnologia (FCT) in the framework of the Strategic Funding UID/FIS/04650/2019 and in the ambit of the project CONCERT (POCI-01-0145-FEDER-032651 and PTDC/ NAN-MAT/326512017), co-financed by the European Regional Development Fund (ERDF), through COMPETE 2020, under Portugal 2020, and FCT I.P. M. Lúcio thanks FCT and ERDF for doctoral position Ref. CTTI-150/18-CF(1) in the ambit of the project CONCERT. This work was further supported by Gilead GÉNESE, Gilead Portugal (refs. PGG/046/2015).

DODAB:MO versus novel liposomes for protein delivery: comparing toxicity and encapsulation efficiency

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Keywords: Liposomes, Dimethyldioctadecylammonium bromide, Monoolein, Encapsulation, Toxicity.

Abstract: Several lipids are used to produce liposomes as nanotechnological solutions for biomedicine (Gauglitz, 2016). Liposomes mimic cell membranes and are interesting in terms of interaction with cells, tissues and organs. However, the features of liposomes are dependent on lipid characteristics, such as amphiphile shape, electrical charge and dependent on their medical application (Li et al., 2019). Our group developed a Dimethyldioctadecylammoniumbromide (DODAB) and monoolein (MO) formulation that was approved for delivery of different biomolecules (Oliveira et al., 2014) and now is being optimized for protein delivery. These liposomes were compared to a novel liposomal formulation, composed by a mixture of 5 different lipids, mimicking vesicles produced by human cells. The purpose of this comparative study was to identify the most suitable formulation for efficient delivery of bioactive cytokines to human cells, with minimal toxicity. Both types of formulations were characterized in terms of size (DLS) and surface charge (zeta potential). Using small quantities of model protein bovine albumin serum (BSA), we optimized the sensitivity of the quantification by the Bradford method, to calculate encapsulation efficiency in both systems. Toxicity was evaluated using *in vitro* animal cell models (MTT assay) and hemolysis assessment (spectroscopy assays). DODAB:MO demonstrated to have higher encapsulation efficiency and moderate toxicity when used in lower lipid concentrations. Nevertheless, novel liposomes demonstrated to be less toxic regardless of lipid concentration and to have lower encapsulation efficiency. In order to adjust the formulation to the intended goal, it is necessary to balance characteristics such as efficiency in cargo loading, delivery and toxicity assessment.

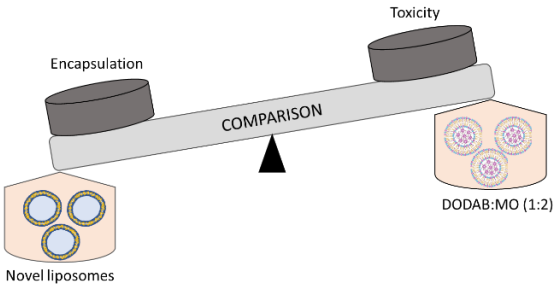

Figure 1 Comparison between encapsulation and cytotoxicity parameters regarding novel liposomes and DODAB:MO formulation.

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Nonlinear optical response of excitons

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Keywords: Nonlinear, Optics, Excitons

Abstract: An exciton is a bound state of a conduction band electron with a valence band hole, that is formed due to the attractive Coulomb interaction between the two particles. This excitation, which exists only in the presence of an external optical electric field, is essential to the description of the optical response of cold semiconductors [1], and in particular, of those that are two-dimensional: the attractive Coulomb interaction is underscreened as no material, and thus no charge, exists in the out of plane direction. Though the standard approach to this problem is based on the Bethe-Salpeter equation (a set of complicated coupled equations in **k**-space), it is possible, under certain approximations, to reduce it to a Schrödinger equation for the Keldysh-Rytova potential, a problem that can be solved using semi-analytical methods [2]. With this method, one can easily compute the relevant objects for the description of the linear and nonlinear optical response: the excitonic eigenvalues and transition matrix elements. The conductivity description that will be presented, which allows for an order by order study of the different nonlinear effects, follows from an analysis of the equations of motion of coherences and populations associated to the excitonic states and gives one a concise (and alternative to [3]) procedure to the derivation of the response functions.

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A graphene-based terahertz plasmonic device for biosensing

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Keywords: Graphene, Microfabrication, Surface Plasmon Polariton, Biosensing, Terahertz materials

Abstract: Infrared spectroscopy (IR) is a powerful technique for identifying biomolecules based on their vibrational spectra[1]. This label-free technique offers biochemical information in a non-destructive way. Nonetheless, IR (3-10μm) and Far-IR, known as terahertz radiation (10-1000μm), interacts poorly with biomolecules (~10nm). This limitation can be overcome by resort to strong optical near fields in the vicinity of resonant metallic nanostructures at the cost of a narrow spectral bandwidth. Graphene provides an ideal platform in this spectral range, offering strong light matter interactions due to its long-lived collective electron oscillations (plasmons) and an unprecedented field confinement[1,2]. In addition, contrary to plasmonic in noble metals, graphene offers tunability by electrostatic gating.

Within the framework of the GRAPHSENS project, several architectures were microfabricated to explore Surface Plasmon Polaritons (SPP) on graphene. The first approach is based on patterning graphene nanoribbons by Electron-beam lithography(Fig1.a). A second approach is based on a continuous graphene monolayer transferred onto a grating of contrasting dielectric materials, such as Si/SiO_2 or Si/air(Fig.1b) with a pitch of 2-4μm. Both architectures are based on theoretical simulations by team members[2,3]. All samples were successfully microfabricated and analysed with a Far-IR to Terahertz source using Fourier-transform IR spectroscopy. With current IR techniques, SPP was not observable on these devices thus we will now try detection using THz time-domain spectroscopy, made by UPorto partners in the project.

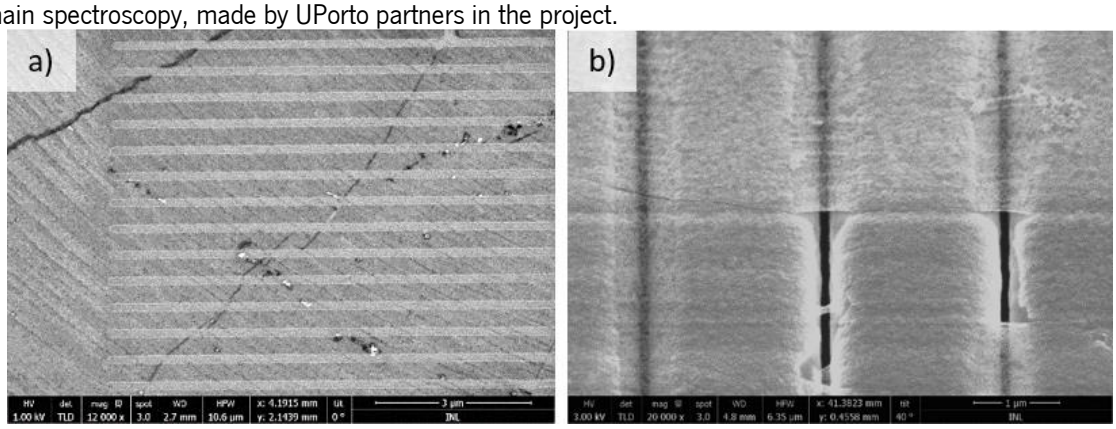

Fig.1. SEM images of: a) Graphene nanoribbons with a pitch of 500nm, and, b) Graphene monolayer on a grating of SiO2 and air.

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Design and Development of Laser Surface Textures to Reduce Friction For Steel

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Keywords: Laser Surface Texturing (LST); Coefficient of Friction (COF); Dimples; Load Carrying Capacity (LCC); Texture.

Abstract: The daunting challenge to overcome the skin-drag-friction in journal-bearing/ball-bearing, piston-ring assemblies, casting/moulding processes and water-going vessels still exists. Friction causes wear and tear, resulting in the dissipation of energy which in turn increasing fuel consumption. Laser Surface Texturing (LST) was used by us to produce textures on steel, copper-beryllium and graphite to overcome this issue. In this work, the target material is steel. Different texture geometries (spherical dimples, rectangular and triangular) and different laser parameters (power, frequency, scanning speed, interspacing and number of passages) were investigated to assess their influence on the frictional behaviour. Eventually, a spherical texture geometry was selected in accordance to the best results presented in the literature. In order to optimize the dimensions of the dimples Finite Element Method (FEM) was utilized. Then the dimensions were confirmed by Scanning Electron Microscopy (SEM). Furthermore, their tribological performance was evaluated by three different friction testing methods namely block-on-ring, line-contact (non- conformal contact) and flat-ring-on-flat (conformal contact). PAO-ISO-VG 46, 150 and 320 (Poly-Alfa-Olefin) lubricating oil was used in friction tests. Texture covered area along with dimple depth to diameter ratios (aspect ratios) were used. The results demonstrate that there is a substantial reduction in the coefficient of friction (COF) up to 28.5% for different speeds. This reduction in the COF improves the Load Carrying Capacity (LCC) for the kinetic pair. To conclude, the dimples we produced by LST reduce friction effectively. Hence, we expect a positive impact on the long-term performance of aforementioned applications with the proposed LST method.

Electroactive polymer-based microstructures for biomedical applications

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Keywords: polymer, electroactive, biomedical, nanoprecipitation, electrospinning

Abstract: Electroactive materials, particularly piezoelectric polymers, have been gaining special attention for biomedical applications due to their ability to convert electric stimuli into mechanical responses, or vice versa [1]. Poly(vinylidene fluoride) (PVDF), its copolymer polyvinylidene-*co*-trifluorethylene (P(VDF-TrFE)) and poly(L-lactic acid) (PLLA) are hydrophobic and biocompatible piezoelectric polymers with high mechanical strength, which can be tailored into distinct morphologies including microspheres and electrospun fibers. Here, PVDF microspheres were obtained using electrospray and similar PVDF-TrFE structures using a nanoprecipitation technique. For electrospray, spheres are obtained by applying an electrical current to the solution, with sizes ranging from 0.81±0.34 to 5.55±2.34 µm [2]. Nanoprecipitation takes advantage of the interfacial deposition of a solvent phase containing the polymer over a non-solvent phase. Sphere diameters vary between 100 and 1100 nm. These spheres have applications in areas such as tissue engineering, particularly in bone regeneration. Electrospinning allows membrane formation for point-of-care (POC) devices, specifically for an alternative for microfluidic paper-based analytical devices (µPADs) [3]. A proof of concept for a glucose detection and quantification test was developed.

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Antifungal action of ZnO thin films prepared by glancing angle deposition

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Keywords: Zinc oxide, Glancing angle deposition, Surface porosity, *Candida albicans,* Antifungal surfaces

Abstract: Thin films of zinc oxide (ZnO) were produced by reactive DC magnetron sputtering with sputtering angles of α = 0°, 40°, 60° and 80° (glancing angle deposition configuration), to be tested against the pathogenic fungus *Candida albicans*. The results showed the formation of stoichiometric ZnO thin films, with inclined columns for incidence angles ≥ 40°. All thin films presented high transparency in the visible range above the bandgap region (near 380 nm). The deposition conditions gave rise to a three-fold increase of the surface porosity with the increment of the incidence angle. Noteworthy, is the formation of different types of pores distributions, from micro-, through meso-, to macropores. Regarding the biological effect, the thin films produced with inclined columns presented a significant antifungal activity, with the inhibition of viable cell growth by 68 %. Moreover, the formation of mesoporous films enhanced the antifungal activity of ZnO thin films against *Candida albicans*. The overall behaviour indicates that these thin films are promising candidates to be applied in antifungal surfaces, as well as to be used in further studies to determine the molecular mechanisms involved in the antimicrobial action of ZnO.

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Development of Clear, Photocatalytic and Self-cleaning Asphalt Mixtures

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Keywords: photocatalytic asphalt mixtures, nano-TiO_2, gas degradation, self-cleaning, clear asphalt

Abstract: Nowadays, there is an increasing concern in transportation engineering about the use of techniques less harmful to the environment and also about road safety. Heterogeneous photocatalysis based on the application of semiconductor materials onto asphalt mixtures is a promising technology because it can mitigate air pollution and road accidents. The functionalized asphalt mixtures with photocatalytic capability can degrade pollutants, such as damaging gases and organic compounds adsorbed on their surface, from specific reactions triggered by sunlight photons. In this research, a transparent binder was used in order to compose an asphalt mixture AC 10 and, for the functionalization, the semiconductor nano-TiO_2 was applied by different methods: spraying coating (with the covering ratios 4, 8 and 16 mg/cm^2), bulk incorporation (3 and 6%) and bitumen modification (0.5, 3, 6 and 10%). All the samples will be tested by gas degradation (e.g. acetaldehyde and NO_x) and soot degradation and compared to the blank samples without semiconductors. It is expected that the samples will be able to degrade a concentration of the gas and also the soot under irradiation of UV light. These tests will also allow the comparison among the application methods of semiconductor. The combination of transparent bitumen and nano-TiO_2 can provide lighter-colored asphalt mixtures mainly for specific applications, such as tunnels, which are very polluted. With the degradation of the gases and the organic compounds, the functionalized asphalt mixtures will provide significant environmental and social benefits.

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Enhanced ionic conductivity in electrospun separator membranes based on poly(vinylidene fluoride) blended with different ionic liquids for lithium-ion battery applications

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Keywords: polymer electrolytes, PVDF, ionic liquid, electrospinning

Abstract: Lithium ion batteries (LIBs) are among the most suitable energy storage systems, due to their high energy density, high operating voltage and long cycle life [1]. Separators are key components in LIBs, functioning as physical barrier between electrodes, allowing simultaneously the ion flow. A good separator/electrolyte must show high chemical stability, high ionic conductivity, high electrical resistance and mechanical strength [2]. Different kinds of fillers, such as ionic liquids (ILs), can be added to the separator structure, in order to improve its properties. Preparation techniques also have significant influence in the separator properties. By using electrospinning to produce fibers, it is possible to increase the superficial area of the membrane, which can increase the battery performance. Electrospun poly(vinylidene fluoride) (PVDF) fiber membranes with different ILs were produced and their potential as separators for battery applications was evaluated. Different types of ILs sharing the same anion, bis(trifluoromethylsulfonyl)imide [TFSI], were used at different IL concentrations between 0% and 15% wt. The morphology, microstructure thermal properties and ionic conductivity of the samples were analyzed. It is shown that the presence of ILs in the PVDF polymer matrix influences the structure and thermal stability of the membranes, as well as their crystallinity. The electrochemical tests showed high ionic conductivity and stability, with good cycling performance at different current rates. Thus, it is proved that the prepared membranes are suitable for applications in separators for lithium ion batteries (LIBs).

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Analytical expressions for the second order conductivity of a cold semiconductor

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Keywords: Nonlinear, Optics, Crystals, Analytical treatment

Abstract: The study of the nonlinear optical (NLO) response in crystals, which dates back to the early nineties [1], has recently resurged as an extremely active research topic. This recent attention is mainly due to: the two-dimensional materials that have been discovered in the past decade can produce exceptionally large nonlinear optical responses; recent studies of topological Weyl semimetals have taken up NLO as a possible probe of the properties of these materials [2]. As such, the development of numerical [3] and analytical tools that allow for the calculation and the understanding of NLO responses is of the utmost importance. Special emphasis should be given to the latter type of tool as it allows one to grasp how a given NLO effect depends on the different physical parameters of the problem (gap, chemical potential, ...). In addition, these expressions should allow one to understand the different processes that are contributing to a given effect, e.g., the injection and shift currents in the photogalvanic response. In this work, we present analytical expressions for the real and imaginary parts of the second order response of cold semiconductors, as well as their application in the study of the response of two different toy models. This application allows for a comparison between results from these new expressions and numerical ones: the agreement between the two is exceptional.

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Magnetic dipolar synchronization of vortex-based spin torque nano-oscillators with independent top contacts

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Keywords: Magnetic tunnel junction, spin torque nano-oscillator, synchronization.

Abstract: This work shows the first results of an ongoing study, regarding the synchronization of vortex-based spin torque nano-oscillators (STNOs) [1]. STNOs are novel nanoscopic microwave oscillators based on spintronic magnetic tunnel junctions (MTJs) [2]. Here, one aims to surpass the major roadblock still preventing the wide spread application of STNOs by integrating and synchronizing an array of STNOs to increase the delivered output power and spectral purity.
A CoFeB/MgO/CoFeB-based MTJ stack was deposited by magnetron sputtering. Circular pillars (diameter, ranging from 250nm to 350nm) were defined by e-beam lithography and ion milling. The free layer has a remanent vortex state. Each STNO has an independent top contact, so that the DC current may be controlled individually. The sustainable oscillation of a single STNO is achieved by applying a sufficiently large DC current and a perpendicular magnetic field [3]. The oscillation frequency is tuned by the DC current [4], so that for a pair of STNOs, the synchronization was attempted by maintaining constant the current of one STNO and sweeping the current of the other [5] and via dipolar interaction, which means that the STNOs were fabricated close to each other [6].
For a pair, i.e. two 350nm pillars 1 μm apart, it is shown that the synchronization is possible in frequency, whereas the power and linewidth are not significantly improved, meaning, not only that a time domain analysis must be performed to know the phase-difference role in the process, but also that the MgO barrier thickness must be optimized.

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(Para)magnetic nanocarriers for early detection and treatment of solid tumors.

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Keywords: Magnetic hyperthermia, Magnetic resonance imaging, Drug delivery, Magnetic nanoparticles.

Abstract: In 2018, there were an estimated 18 million new cases of cancer in the world with more than 9 million deaths. The vast majority of these cancers appear as solid tumours. Current treatment protocols are still far from being the solution to this problem. Therefore, an innovative tool against solid tumours was developed through a combination of early diagnosis and treatment (theranosis).
We have recently developed a multifunctional nanocomposite including magnetic nanoparticles (MNPs) dispersed in a lipid matrix. The lipid part of the system can be used to encapsulate chemotherapeutic agents increasing the local concentration of the drug in the cells, and protecting healthy tissues from the deleterious effect of the drug, reducing side effects. MNPs have been translated to the clinics as magnetic resonance imaging (MRI) contrast agents (CAs) and thus can be used for the early non-invasive detection of tumours. MNPs can as well be used to generate heat under alternating magnetic fields, that can be used for the direct ablation of tumours through hyperthermia, and/or for the externally controlled delivery of drugs.
This study aims for the creation of a nanocomposite containing a chemotherapeutic drug, doxorubicin, and a (para)magnetic core made of magnetite (Fe_3O_4) NPs and manganese oxide (MnO) NPs. The nanocomposite was characterized in terms of physico-chemical and functional properties and validated *in vitro*, presenting a great performance as an MRI contrast enhancer, MH effector and controlled drug delivery system. Overall this formulation showed potential to work as theranostic agent in the fight against cancer.

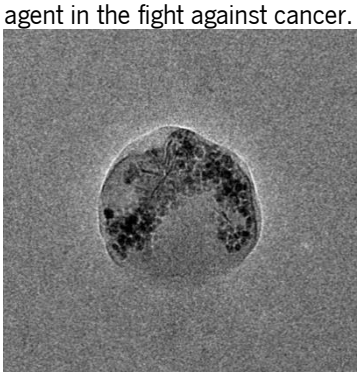

Figure - TEM micrograph of a nanocarrier containing a paramagnetic core (SLN@MnO-Fe_3O_4).

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Fluorescent Effect on Textile Supercapacitors

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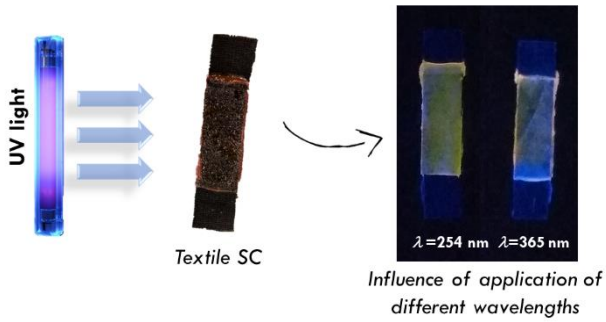

Keywords: textile supercapacitors, fluorescence, energy storage, carbon-based nanomaterials

Abstract: In a society continuously motivated by new electronic technologies with advanced functionalities, there is a strong demand to develop miniaturized and efficient energy storage systems. One solution involves the development of supercapacitors (SCs), due to their unique properties such as fast charging, high cycle life and eco-friendly nature [1]. In particular, most of the textile SCs developed so far present in their composition carbon-based materials due to their conductive properties. However, this type of devices typically presents a dark color, which limits its applications in fashion.

In this work, materials with electrical and luminescent properties have been used in order to develop multifunctional electronic devices that simultaneously present the ability to store energy and a response to the action of UV light. To achieve that goal, textile substrates were coated with a conductive carbon nanomaterial (CC) and a fluorescent pigment (FP), and then used for the production of a textile SC (SC_CC_FP). For comparison, a device without fluorescent pigment (SC_CC) was also produced. Several characterization techniques were performed including XRD, FTIR-ATR and SEM-EDS, confirming the successful preparation of the functionalized textiles. Both textile devices presented an electrical double layer capacitive behavior, but SC_CC_FP also suggested the occurrence of redox reactions. SC_CC_FP presented a specific capacity of 4.5 F g^{-1} *vs.* 5.1 F g^{-1} for SC_CC, at 1 mV s^{-1}. In terms of internal resistance, the SC_CC_FP present variations between 259.5 Ω and 331.4 Ω. On the other hand, SC_CC sample showed a continuous decrease of its value upon the variation of the light wavelength (λ = 254 nm, 365 nm or visible light). The energy and power density values were approximately 1.75 W h kg^{-1} and 1074.2 W kg^{-1}, showing improvements in the power density value compared to 2.26 W h kg^{-1} and 624.9 W kg^{-1} for SC_CC. The exposure of the SC_CC_FP to UV light also resulted in a color change from black to orange, thus showing versatility for fashion applications.

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Orbital Hall effect in Transition Metal Dichalcogenides monolayers

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Keywords: Orbitronics, transition metal dichalcogenides, two-dimensinal materials, electronic transport

Abstract:The field of spintronics blossomed in the last decade, as a consequence of the use of spin-orbit coupling to generate and manipulate spin currents in non-magnetic materials. In these systems, the efficient conversion between charge and spin currents is mediated by spin-orbit. Great progress in the manipulation of the orbital angular momentum of light has also been achieved in the last decades, leading to a large number of relevant applications. Still, electron orbitals in solids were less exploited, even though they are known to be essential in several underlying physical processes in material science. The orbital-Hall effect (OHE), similarly to the spin-Hall effect (SHE), refers to the creation of a transverse flow of orbital angular momentum that is induced by a longitudinally applied electric field. The OHE has been explored mostly in metallic systems, where it can be quite strong. However, several of its features remain unexplored in two-dimensional (2D) materials.

We investigate the OHE in multi-orbital 2D insulators, such as transition metal dichalcogenides monolayers and show that the OHE in these systems is associated with exotic momentum-space orbital textures. This intrinsic property emerges from the interplay between orbital attributes and crystalline symmetries and does not rely on the spin-orbit coupling. Our results indicate that multi-orbital 2D materials can display robust OHE that may be used to generate orbital angular momentum accumulation, and produce strong orbital torques that are of great interest for developing novel spin-orbitronic devices.

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Self-assembling of dipeptide nanotubes inside electrospun fibers with strong piezoelectric response

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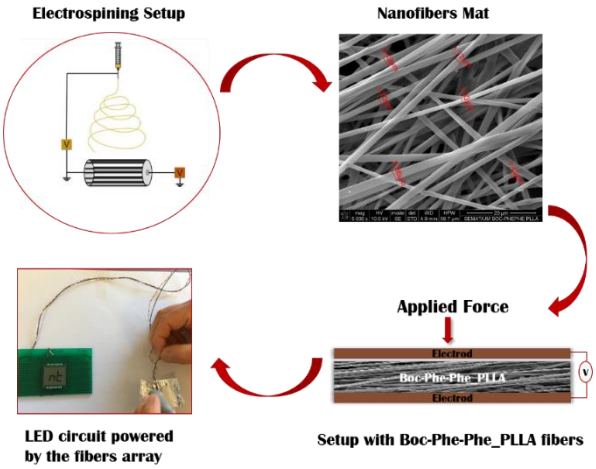
Keywords: functional nanofibers; dipeptide self-assembling; piezoelectricity; electrospinning

Abstract: Dipeptide biomaterials are strong piezoelectric materials that can convert applied mechanical forces into electricity. We have developed large-scale hybrid electrospun arrays containing N-tert-butoxycarbonyl (Boc) diphenylalanine under the form of nanotubes embedded in biocompatible polymers. These nanofibers exhibit strong piezoelectric properties when a periodic mechanical force is applied. The nanostructured hybrid materials were produced by the electrospinning technique. Optical absorption measurements show four bands in the spectral region 240-280 nm indicating quantum confinement due to nanotube formation of Boc-diphenylalanine in dichloromethane solutions. A strong blue photoluminescence emission was observed from nanotubes crystallized inside the fiber arrays during the electrospinning process. These two dimensional hybrid biomaterial structures are able to generate voltage, current and density power of up to 30 V, 300 nA and 2.3 μWcm^{-2}, respectively, when applied a periodical force of 1.5 N.



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Enhancing the performance of separator membranes by surface micropatterning for lithium ion batteries

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Keywords: PVDF-TrFE, patterned surface, membrane, lithium-ion battery, polymer separator

Abstract: The rapid development of technology and growing mobility contribute to the need for new ways of energy generation and store [1]. Lithium primary cells are widely used for portable electronics, being increasingly important for the new generation power sources taking into account their advantages: lighter, cheaper, higher energy density, no memory effect, higher number of charge/discharge cycles when compared to other battery technologies.
One key element in lithium-ion battery systems is separator membrane placed between the electrodes. Separator membranes should show high ionic conductivity, excellent mechanical properties, good chemical stability and controlled porosity, poly(vinylidene fluoride) (PVDF) and (vinylidene fluoride) (VDF) copolymers such poly(vinylidene fluoride – co – trifluoroethylene) (PVDF-TrFE) being widely used for this application [2].
The goal of this work is evaluated the effect of different patterned surfaces based on poly(vinylidene fluoride-cotrifluoroethylene) (PVDF-TrFE) constituted by arrays of hexagons, lines, zig-zags and pillars microstructures on battery performance and correlate with its morphology. Also, computer simulations allow to deeper understate the influence of the patterned surface on battery response.
Discharge capacity of batteries with zig-zag micropatterned separators is the highest among the patterned separators, 804% higher than the one for batteries with non-patterned separators

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Ionic Liquid based polymer actuators

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Keywords: electroactive materials, ionic liquids, polymers, sensors and actuators

Abstract: The development of ionic electroactive materials based on the combination of polymers with ionic liquids (ILs), has emerged as a promising approach in the field of sensors and actuators. ILs are defined as molten salts at room temperature with unique and interesting properties (negligible vapor pressure and high ionic conductivity (~10^{-3}-10^{-2} Scm^{-1}), among others) [1]. Poly(vinylidene fluoride) (PVDF) presents the highest electroactive properties among polymers, being the β phase the main responsible for its piezoelectricity. The properties of ionic electroactive materials can be tailored through the IL type (cation and anion nature), IL content and polymer matrix. Further, also sustainable sensors and actuators based on natural derived polymers such as cellulose and silk can be produced [2,3].

In this work, ionic polymer actuators based on different polymers matrixes (PVDF, cellulose and silk) containing ILs will be presented. The effect of the IL cation alkyl chain size on the PVDF based actuator performance has been evaluated, being the highest bending response observed for [Pmpip][TFSI] composites (where Pmpip represent propylmethylpiperidinium): 6.0 mm at 5 V and 100 mHz. Sustainable actuators based on 2-hydroxy-ethyl-trimethylammonium dihydrogen phosphate ([Ch][DHP])/silk and [Ch][DHP]/sodium carboxymethyl cellulose (NaCMC) composites show displacements above 8 mm and 9 mm, for applied voltages of 5 and 8 V, respectively. Additionally, the potential of the developed materials for printable sensors will be presented.

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Transparent magnetoactive composites

R. Polícia[1], A. C. Lima[1,2], N. Pereira[1,3], E. Calle[4], M. Vázquez[4], S. Lanceros-Mendeza[5,6] and P. Martins[1,7,*]

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Keywords: magnetoactive, smart materials, composites, microwires, magnetoelectric

Abstract: Polymer-based magnetoelectric materials changed thinking in advanced and multifunctional materials research some years ago. The design and application of magnetoelectric multifunctional materials with specific microstructures included the biomedical field, energy harvesting, sensors and actuators, among others [1].
In this context, the development of optically transparent multifunctional magnetoelectric (ME) materials will open the range of applications to new directions such as transparent sensors, touch display panels, multifunctional flat panel displays and optical magnetic coatings.
This work introduces the first flexible and transparent ME composite, composed of P(VDF-TrFE) and Fe72.5Si12.5B15 microwires (exhibiting a magnetic polarization of 1.5T) and a maximum ME voltage response of 65 $mV.cm^{-1}Oe^{-1}$, obtained at the critical longitudinal applied field of at 14500 $A.m^{-1}$, having in this way, the higher (ME voltage)/(DC magnetic field) ratio reported in the literature. The origin of this high coupling is explained and related with the transversal anisotropy of the microwire.
Such features allow us to anticipate the use of the developed materials on a new generation of transparent electronics and magnetic devices.

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Environmental remediation strategies based on polymernanocomposites

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Keywords: Adsorption, nanomaterials, photocatalysis, membrane, and water remediation

Abstract: Conventional wastewater treatment plants are ineffective in the removal of emerging pollutants from the water. Thus, photocatalysis may be an alternative since it allows their rapid and efficient removal from water, transforming them into harmless by-products. Among several semiconductor materials, titanium dioxide (TiO_2) is the most widely used for the degradation of organic pollutants, owing to their physical and chemical stability, low cost, and unique electronic and optical properties.
This work presents different approaches to overcome these drawbacks, namely the recuperation and utilisation of the nanocatalysts, the enhanced photocatalytic activity under sunlight and the potential toxicity of the catalytic material and degradation by-products. Strategies for improving photocatalyst efficiency includes rare earth doping, decoration with gold nanoisland and the preparation of composites with graphene and graphene oxide. Immobilisation has been achieved in electrospun mats, porous membranes and coatings, allowing recuperation and re-use of the materials. Adsorption processes and multifunctional materials are were also developed to tackle a wider range of environmental pollution such as heavy metals (Arsenic), and water disinfection and enlarge the life span of membranes (reduce fouling).

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Ground state phase diagram of spin-1/2 transverse ANNNI chain

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Keywords: Axial nearest and next nearest neighbour Ising chain, phase diagram, quantum discord, entanglement of formation.

Abstract: This talk focuses on the ground state phase diagram of a one-dimensional spin-1/2 quantum Ising model with competing first and second nearest neighbour interactions known as the ANNNI model in the presence of a transverse magnetic field. Due to contradictory results obtained by different approaches, there is no clear picture of its phase diagram at zero temperature. Here, using numerical and analytical approaches, some important evidence is provided which is helpful to clarify the identification of the ground state phase diagram. According to numerical Lancsoz results, the critical lines and the order of phase transitions are determined by the study of some proper ground state functions and quantum correlations of the system. All studied quantities identify the two ferromagnetic-paramagnetic
and antiphase-floating boundary lines. Quantum correlations play a crucial role in the detecting of two other phase transitions. The Peschel-Emery one-dimensional line can be identified by the quantum discord and its derivative. The entanglement of formation is also the only quantity able to magnificently reveal the fourth boundary line regarding the floating-paramagnetic phase transition.

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