

Jornadas 2019

VII Annual Meeting

14/12/2019

INSTITUTE FOR
NANOSTRUCTURES,
NANOMODELLING AND
NANOFABRICATION

RESEARCH, INNOVATION AND
ENGINEERING APPLICATIONS

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FACULDADE DE
CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA



Programme

JORNADAS 2019

Friday 13 Dec 2019

17h 00m

National Coordination Meeting (CICFANO)

Saturday 14 Dec 2019 **Morning**

09h 30m

Registration / breakfast DeCA Hall)

09h 30m – UA members

10h 00m – UNL members

10h 30m

Opening Session (Auditorium CCCI - DeCA)

Prof. João Veloso (i3N | UA Coordinator)

Prof. Artur Silva (Vice-rector, UA)

Profª. Elvira Fortunato (i3N Coordinator, Vice-rector UNL)

11h 00m

Posters Pitch – (3 min. x 28)

12h 45m

Lunch Time

Castro University Restaurant

Saturday 14 Dec 2019 **Evening**

14h 00m

Posters Session (DeCA Hall)

14h 45m

Invited Plenary by Professor Pablo Ordejón, Director of ICN2 (Auditorium CCCI - DeCA)

15h 45m

i3N Group presentations (15 min each)

João Pinto (NO)

João Borges (SBMG)

Ricardo Dias (TCP)

João Veiga (ME)

João Veloso (PAMD)

Rodrigo Martins (MEON)

17h 30m

Coffee break (DeCA Hall)

18h 00m

Posters Summary by Prof. Rodrigo Martins (Auditorium CCCI - DeCA)

18h 30m

Announcements

Awards:

- i3N publications with the highest Impact Factor

- Best Poster

19h 00m

Closing Session

P1: **"Theory of Defects in Semiconductors: Bulk, Surfaces and Nanostructures"** by: José Coutinho

P2: **"Cellulose-based Hydro-responsive Materials"** by: Ana Almeida

P3: **"Topological Insulators: symmetries, interactions and bound states"** by: Anselmo Marques

P4: **"Development of multifunctional electrospun magnetic membranes for biomedical applications"** by: Paula Soares

P5: **"Structural Properties of Complex Networks"** by: Gabor Timar

P6: **"Solution-based Zinc-Tin Oxide nanostructures: from synthesis to electronic applications"** by: Ana Rovisco (Jorge Martins)

P7: **"Structure and Dynamics of Biological and Social Networks"** by: Edgar Wright

P8: **"Ancient Bronze production technologies: from Cu & Sn ores to metals"** by: Elin Figueiredo

P9: **"Nanostructured ZnO and ZnO/nanocarbon composites for biosensing applications"** by: Joana Rodrigues

P10: **"Multifunctional and transparent low cost metal oxide electronics"** by: Emanuel Carlos

P11: **"IFLUX- X-ray Fluorescence Imaging based on Micro-patterned Gaseous detector"** by: Ana Luísa Silva

P12: **"Cements and Mortars in Historical Monuments: Contributions for the Preservation of Built Cultural Heritage"** by: Fernanda Carvalho

P13: **"Novel optical fiber sensor designs for AROMA compounds detection"** by: Marta Ferreira

P14: **"TCAD simulation platform for oxide transistors and memories"** by: Jorge Martins

P15: **"Electrical transport mechanisms in Ta2O5-based memristive devices"** by: Carlos Rosário

P16: **"Design of nanoSERS platforms for biosensing"** by: Maria João Oliveira

P17: **"Crystalline silicon nanoparticles for new (opto)electronic applications"** by: Bruno Falcão

P18: **"Cellulose Photonic Circular Polarized Light Detectors"** by: Paul Grey

P19: **"Graphene foams and membranes for electromechanical sensing"** by: Alexandre Carvalho

P20: **"Magnetic bioactive glass-based 3D systems for bone cancer therapy"** by: Ricardo Matos

P21: **"Investigation of ferroic nanostructures for energy and environment"** by: Venkata Ramana

P22: **"Solution Processed Halide Perovskite Thin Film Transistor"** by: Santanu Jana

P23: **"Developing Biomaterials and Ceramics for Industrial Applications"** by: Sílvia Gavinho

P24: **"Design of optimized photonic microstructures coupled with luminescent down-shifting for high-efficient, flexible and stable perovskite solar cells"** by: Sirazul Huque

P25: **"Optical fiber sensors networks for in situ lithium-ion batteries monitoring"** by: Micael Nascimento

P26: **"Nanoscale data storage by Probe Induced charge injection method"** by: Suman Nandy

P27: **"Development and optimization of optical fibre sensors by a femtosecond laser"** by: Tiago Paixão

P28: **"Structurally colored bio-inspired sustainable materials"** by: Susete Fernandes

Theory of Defects in Semiconductors: Bulk, Surfaces and Nanostructures

J. Coutinho*, V. J. B. Torres, P. Santos, J. D. Gouveia

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We present a showcase for our research activities regarding defect-related problems, mostly in semiconductors (in bulk, their surfaces, alloys and nanostructures), but also in other materials like oxides or biological minerals. Our approach involves first-principles atomistic modeling techniques, many-body perturbation methods and classical molecular dynamics. Among our recent works, we single out: (i) The investigation of defects responsible for trapping carriers in ultra-hard radiation detectors based on silicon carbide (SiC) Schottky diodes [1]; (ii) Finding and understanding the mechanisms of optically addressable spin states localized on defects suitable for quantum-bit storage [2]; (iii) Unveiling the defect behind the light-induced degradation of silicon-based solar cells [3]; (iv) The atomistic and electronic structure of semiconductor strained surfaces and steps [4], (v) The optical and magnetic functionalization of hydroxyapatite, a constituent of bones and teeth, by means of defect engineering [5], and (vi) The dynamics of phonons and polaritons in semiconductor alloys by combining first-principles modeling with Raman spectroscopy [6].

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Cellulose-based Hydro-responsive Materials

A. Almeida¹, P. Silva¹, F. Gonçalves¹, J. Canejo¹, P. Almeida^{1,2}, M. Godinho^{1*}

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Humidity-driven movements observed in plants are an inspiration to design cellulose biomimetic materials. These movements are observed in dead plant tissues, namely in awns that transport seeds, and are attributed to anisotropic cellulose-based micro/nano structures organized to change shape upon environmental conditions, for example water content, activated by humidity changes.[1] Here we report on a simple and efficient strategy to isolate cellulose-based hygroscopic responsive materials from *Erodium* awns dead tissues, a representative of the Geraniaceae family, which change from twisted to rod like shapes upon wetting. A stimuli-responsive material was isolated, it forms left-handed (L) or right-handed (R) helical birefringent transparent ribbons in the wet state that reversibly change to R helices when the material dries. The possibility of actuating chirality via humidity suggests that these cellulose-based skeletons, which do not require complicated lithography and intricate deposition techniques, provide a diverse range of applications that spans from intelligent textiles to micro-machines.[2]

In summary, we have isolated, chemically modified and characterized a helical cellulose based responsive material that can reversibly respond to a variation in hydration with a change of chirality, to the best of our knowledge a hitherto unobserved phenomena that could lead to novel smart material applications.

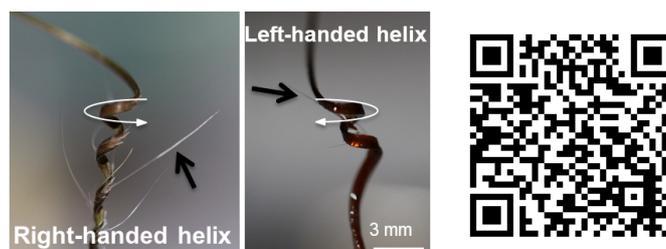


Fig. 1. Chirality Inversion after alkali treatment. The black arrows indicate the hairs of the awn outside and inside of the helical ribbon that form the awn before and after treatment, respectively. QR code of the movie of the hydration of an awn in an alkali water solution (5% w/w) (speed: 8x).

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*Presentation ID: P3**Type of Presentation: Poster*

Topological insulators: symmetries, interactions and bound states

A. M. Marques^{1*}, F. D. R. Santos¹, L. Madail¹, R. G. Dias¹, G. Pelegrí², J. Mompart², V. Ahufinger² and A. J. Daley³

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The established expressions for computing the topological properties of 1D models with inversion-symmetry rely implicitly on having an inversion-axis centered within the unit cell. We show that there are models where the inversion-axes never cross the center of any chosen unit cell. This is shown to entail corrections to the usual expressions for the Zak's phase, polarization, inversion-operator, etc. [1].

For non-interacting models, the topological indices are associated with the properties of the bulk eigenstates in k -space. On the other hand, the bulk-periodic eigenstates of many-body interacting systems cannot be found due to a broken translational symmetry, prompting alternative routes to define the topological indices. Through the study of two-body states in the Su-Shrieffer-Heeger model, we show that certain effective [2] and exact [3] mappings to higher-dimensional single-particle models can be performed where, at the level of these mapped models, the usual topological characterization applies, which in turn allows us to characterize the original interacting model by reverting the mappings.

Finally, an overview of related works in topological systems carried out in collaboration with members from other groups is also provided here [4-6].

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Development of multifunctional electrospun magnetic membranes for biomedical applications

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Design, research and development of new and improved smart structures and systems is currently a hot topic in materials science and engineering. Electrospinning is a versatile and easy to scale-up strategy to produce membranes. Combination of thermoresponsive polymers with magnetic nanoparticles (mNPs) originates dual-stimuli responsive systems, able to change their morphological and chemical properties in response to temperature and magnetic field. This work focuses in developing a dual-stimuli responsive device composed of MG with mNPs incorporated into polymeric fibers as a new cancer treatment option. To produce these dual-stimuli responsive systems different architectures can be designed: thermoresponsive electrospun fibers with mNPs incorporated; or thermoresponsive MG with mNPs confined in polymeric fibers through colloidal electrospinning.

Superparamagnetic iron oxide NPS with an average diameter of 10 nm were incorporated in PNIPAAm MG producing dual-stimuli responsive MGs [1-4]. PNIPAAm MG were incorporated in PEO nanofibers (average diameter of 63 nm) through colloidal electrospinning with a “bead-on-a-string” morphology. Hybrid dual-stimuli responsive MG were incorporated into thermally crosslinked PVP fibers producing a reinforced system able to swell about 10x their weight and to generate 1.5 °C with only 20 mg of composite membrane for 10 min of alternating magnetic field application. In a different approach, mNPs were incorporated into thermoresponsive (polyacrylamide) and non-thermoresponsive (cellulose acetate) polymeric fibers, demonstrating that it is possible to incorporate mNPs into different polymers, thus producing electrospun membranes for magnetic hyperthermia applications [7].

More interesting results are being achieved under the recently financed project DREaMM (Ref. PTDC/CTM-REF/30623/2017) to engineer dual-stimuli responsive magnetic nanofibrous membranes as controlled drug release systems and magnetic hyperthermia agents for cancer treatment.

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Structural Properties of Complex Networks

J. F. F. Mendes¹, S. N. Dorogovtsev^{1,2}, A. N. Goltsev^{1,2}, A. L. Ferreira¹, G. J. Baxter¹, G. Timár¹, R. A. da Costa¹

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We investigate fundamental properties of complex systems that can be derived from the structure of interactions of the constituents. Of primary importance in most systems is the ability to sustain cooperative, ordered states, and the prerequisite for this is that the underlying interaction network is in the “percolating phase” according to some definition of connectivity. Using tools from graph theory and statistical physics we study a wide range of percolation-type phase transitions on different classes of complex networks.

Our main focus in recent years has been on multiplex and interdependent networks that allow for an informative and versatile way of modelling real complex networked systems [1,2,3]. We studied the structural properties of directed networks in general and introduced a novel scheme for their topological characterisation [4]. Another branch of our work deals with optimisation-based network connectivity: we have obtained various important results in describing the phenomenon of explosive percolation [5,6]. We have also made significant advances in the understanding of threshold models such as bootstrap and k-core percolation [7,8].

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Solution-based Zinc-Tin Oxide nanostructures: from synthesis to electronic applications

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Zinc-tin oxide (ZTO) is a multifunctional material being widely studied over the last years. It has already been used for different applications such as photocatalysis, electronics, sensors and energy harvesting. Nowadays, these applications have an even higher importance, specially if we have in mind sustainability. For this reason, ZTO has even more impact since both zinc and tin are abundant, recyclable and environmentally friendly. The current trend in technology is to minimize the devices' size, while looking for smart and multifunctional objects. In this context, nanostructures appear as an important tool for an upcoming generation of transparent nanodevices. ZTO has two crystalline phases, Zn_2SnO_4 and ZnSnO_3 , and for both it's possible to obtain different morphologies, being, however, hard to control the synthesis, due to the presence of two cations. In this work a seed-layer free hydrothermal synthesis was optimized to achieve different ZTO nanostructures, with special emphasis on ZnSnO_3 nanowires (Fig. 1a). [1][2] Structural, morphological, optical and electrical properties were studied, and the multifunctionality of these structures was explored, with very promising results being achieved for energy harvesting devices, resistive switching memories and photocatalysis (Fig. 1b).

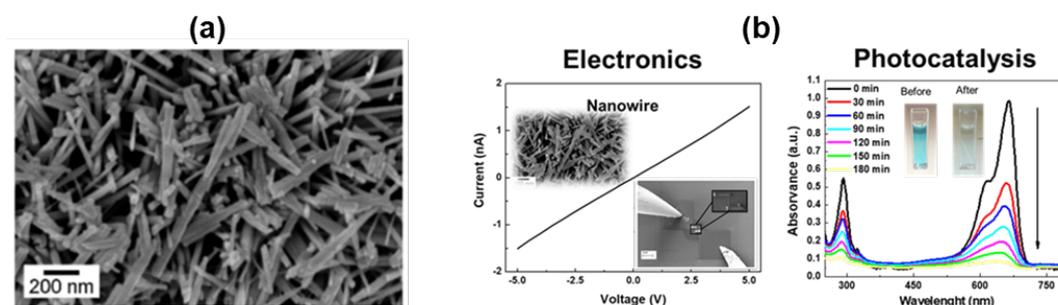


Fig. 1. (a) SEM images of the fabricated ZnSnO_3 nanowires. (b) Examples of applications explored (electronics and photocatalysis).

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Structure and Dynamics of Biological and Social Networks

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Network theory offers an approach to the study of complex systems, composed of many interacting parts, which often display emergent dynamics. Once abstracted onto networks, systems such as regions of the central nervous system, composed of neurons linked by synapses [2, 3], or the Twitter Follow Network [1], can be studied as topological objects. The structural properties of such biological and social networks can then be analysed, with the aim of understanding their impact on dynamical processes that take place in these systems [1, 2, 3, 4, 5, 6, 7]. For example, the global organization of any directed network can be described by the bow-tie diagram, depicted in Fig. 1. Thus, the ability of systems abstracted onto directed networks to support emergent states, such as synchronization – a vital process in biological systems – is determined by bow-tie structure. In particular, the number of SOURCE nodes and links between the IN component and the CORE can mean the difference between synchronization or no synchronization [1].

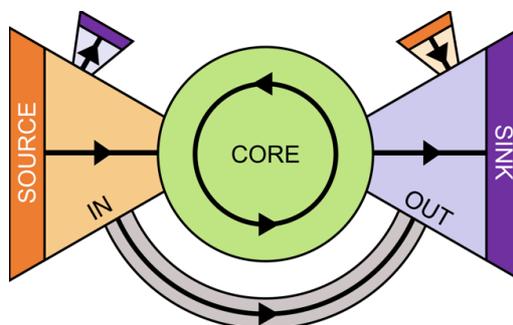


Fig. 1. Bow-tie structure of directed networks [1].

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Ancient Bronze production technologies: from Cu & Sn ores to metals

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Tin was a very important alloying element for the production of bronze (Cu-Sn) since the 2nd millennium BC (Bronze Age). NW Iberia is one of the largest regions with tin resources in Western Europe. Within the project IberianTin (PTDC/HAR-ARQ/32290/2017, Ancient production, uses and circulation of tin in NW Iberia, coordinator Elin Figueiredo), we are investigating archaeological vestiges of ancient mining, tin and bronze technologies of production and we are finding new evidences of tin processing of high international relevance.

While classical bronze composition was set up at c. 10 wt.%Sn, bells, which began to be used in ancient times, were frequently made of bronze with a specific composition (20-25 wt.%Sn) (Fig. 1). Within the project Singing Bronze, an award by Santander Totta/Nova (coordinator at FCT-NOVA Rui J.C. Silva), we are studying the composition and microstructure of historical bells, including the carrillons of Mafra Palace, investigating its relation to bell size and conservation state.

Recently, and within the grant CEECIND/01558/2018 (Assistant Researcher) I was awarded with, we will also be taking gold, namely the simultaneous presence of gold and tin sources in NW Iberian and its uses in gold jewelry, namely in filigree, a production technique that dates back to Iron Age and has become a Portuguese brand image.

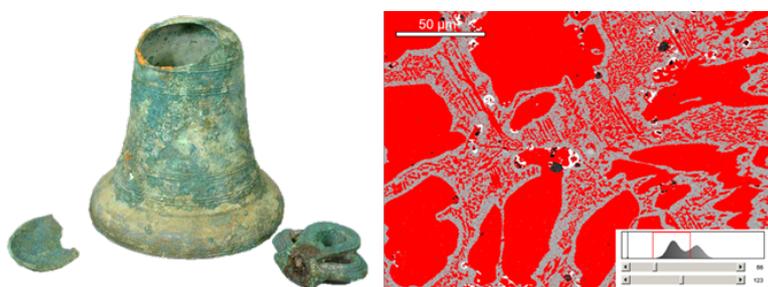


Fig. 1. Image of Coruche bell and OM image of its bronze microstructure (red: Cu rich-phase; grey: Cu_31Sn_8 -phase; white: Pb; black: pores).

Nanostructured ZnO and ZnO/nanocarbon composites for biosensing applications

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Zinc oxide (ZnO) is one of the most versatile semiconductors, having one of the richest varieties of nanostructures, which can confer different functional behaviours. At the nanoscale, the formation of ZnO composites with other materials can alter the properties of both components, giving rise to advantageous properties. Among these composites, the mixture with carbon derivatives (*e.g.* graphene) has been employed in the fabrication of several devices, including biosensors, due to the possibility of achieve enhanced sensing performances. In this research project, we propose the production of ZnO nanostructures and ZnO/nanocarbon composites to be used as transducer material for the detection of environmental and biomedical analytes. These materials are being produced by innovative and up-scalable laser processing techniques [1,2] to be used as transducer platforms capable of combine both optical and electrochemical transduction in the same device, taking advantage of the strong luminescence properties of ZnO and the high electrochemical activity of both components. This combination is expected to allow enhanced data acquisition and counter-proof measurements in a single sample/device, minimizing false-positives and detection errors.

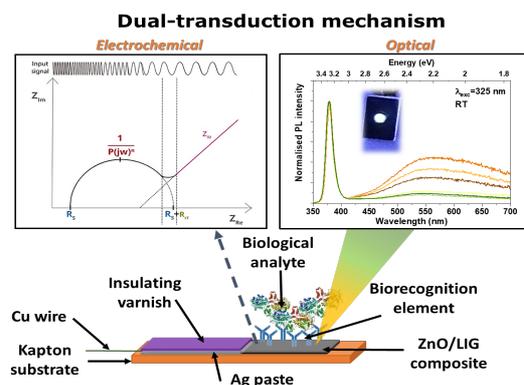


Fig. 1. Schematic representation of the main objective of the project: dual-transduction biosensors.

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Multifunctional and transparent low cost metal oxide electronics

E. Carlos, R. Branquinho*, R. Martins and E. Fortunato**

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Printed electronics have led to new possibilities in the development of low-cost and low-temperature methods for materials production and processing. Inorganic oxide devices that are totally solution-processed offer an appealing approach, overcoming some limitations of organic electronics, such as performance and stability. Solution processed dielectric oxides are a vital part of electronic devices and requirements on film quality and characteristics make their development a challenging task.

Solution processes are simple and versatile however, there are still some drawbacks that need to be addressed. Currently, synthesis of these materials usually needs higher temperatures and longer annealing time which limits their use on flexible substrates which is crucial for flexible and wearable device applications. In this work, a new approach to the production of low temperature and optimized dielectric materials and their application in printable electronic devices will be presented.[1–3]

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IFluX - X-ray Fluorescence Imaging based on Micro-patterned Gaseous detector

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X-rays are assumed to be a very powerful tool in analytical techniques in several fields. When large detection areas with resolution in position and energy are needed, micropatterned gaseous detectors (MPGDs) are an interesting and unique solution in some cases [1].

The main goal of this project is to develop a large area system for energy dispersive X ray fluorescence imaging (EDXRFI) based on MPGDs. The “holy grail” of EDXRFI is acquiring elemental images of areas larger than the probe beam spot size, thus, the use of a large area elemental imaging MPGD can be an elegant approach for a long standing problem.

A micropatterned gas detector will be applied for elemental identification and mapping on samples using EDXRFI [2]. In addition to the main objectives, we expect to raise new questions and challenges related to the development of detectors and associated technologies and contribute positively to the advancement in the fields of biomedicine research [2], material sciences, cultural heritage and also to the industry domain and radiation detectors for imaging.

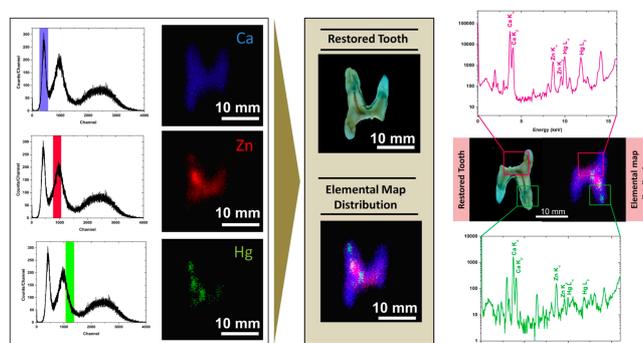


Fig. 1. Biomedical application example : Mercury toxicology - Teeth restored by dental amalgam [2]

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Cements and Mortars in Historical Monuments: contributions for the preservation of built Cultural Heritage

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The societal impact of historical constructions has generated an increased interest in the scientific community, promoting innovative approaches to issues raised by the necessity of preserving cultural assets for the future. Materials Science has an unquestionable role in this approach by developing strategies and methodologies, crosslinking different aspects related to cultural heritage materials, attaining a better comprehension on their properties and historical applications, disclosing correlations and interactions between materials with different origins and supporting a compatibility evaluation with new and improved materials in the context of qualified interventions on built heritage. The materials under study in this work are cements and mortars from different periods of manufacture, corresponding to three important monuments escaping traditional regional constraints: the Monastery of Alcobaça in Portugal, the Palace of Knossos in Greece and the Roman Aqueduct of Carthage in Tunisia. Cements and mortars, used with different functions in historical buildings, may present several problems that affect their structural application and their behavior with adjoining materials. Through and holistic approach to the study of their chemical and physical properties, their interaction with different substrates, their compatibility with different materials and the influence of human and environmental factors for their conservation status, will fulfill the prospect of contributing to preservation strategies of each specific monument encompassing a global outreach of cements and mortars applied to monuments of European origin.



Fig. 1. Issues in materials in Built Cultural Heritage

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Novel optical fibre sensor designs for AROMA compounds detection

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The AROMA project addresses the challenge of detecting aroma compounds using purpose designed optical fibre sensors. It is a project of multidisciplinary nature, with a potentially large socio economic impact, as it involves the development of new tools that can help the quality control processes in industry. The optical fibre sensors will be modelled, fabricated and characterized by following a well defined plan. In a first stage, the detection of single volatile organic compounds will be addressed, and the sensor will be optimized to meet the required specifications. Besides, the detection of Madeira wine ageing markers will also be addressed and the comparison with classical analytical methods will be performed. Furthermore, the concept of lab-on-fibre will be validated, by creating a sensing platform in a single optical fibre enabling the simultaneous measurement of several parameters. An example of one of the lab-on-fibre designs to be explored is shown in Fig. 1. Finally, the platform will be integrated in a lab scale prototype.

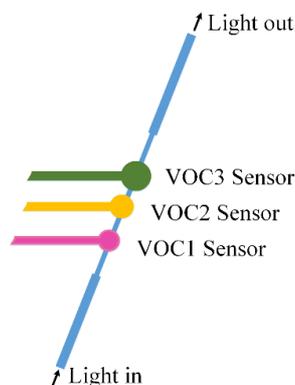


Fig. 1. Schematic design of the proposed lab-on-fibre scheme, based on three microspheres coupled to a fibre taper.

TCAD simulation platform for oxide transistors and memories

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Oxide semiconductor TFTs have been crucial to set transparent electronics as a disruptive and sustainable technology to face future ICT needs. Besides transparency these devices offer low temperature processing, large area uniformity and excellent performance. Similarly, oxide memristors appear as promising candidates for the future RRAM technology, allowing for the same oxide advantages. Still, oxide devices performance and stability need to be improved before it enables fully transparent/flexible, complex/fast, low-cost electronics. TCAD tools for modelling and simulation of oxide devices at a physical level, supported by physical parameter extraction from fabricated devices, is a viable tool in understanding the physical mechanisms behind device operation, which is crucial for further enhancement of device performance and stability. In the current work, this simulation was employed to investigate non-idealities seen on fabricated IGZO devices, namely short-channel effects such as the drain-induced barrier lowering, charge sharing and the channel length modulation), or other effects such as the hump-like behavior in transfer curves[1]. Additionally, TCAD simulation was also used to explore different TFT architectures such as dual gate devices with different second gate biasing conditions (Fig. 1) and other more complicated floating-gate architectures [2].

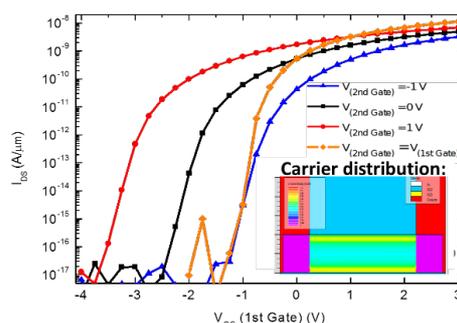


Fig. 1. Simulation of a dual-gate TFT showing the effect of biasing conditions for the second-gate.

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Electrical transport mechanisms in Ta₂O₅-based memristive devices

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Ta₂O₅-based memristive devices show good prospects for the implementation in storage class memory and neuromorphic computing architectures. The resistive switching in such devices is based on the nonvolatile change of the resistance via the modulation of the oxygen content in conductive filaments. However, the filaments' structure and exact composition are still a matter of debate.

We targeted these questions by performing a detailed study of the electronic transport through conductive filaments in Ta₂O₅-based memristive devices at temperatures from 300 K down to 2 K. We then sputtered thin films of TaO_x with different oxygen concentrations and pure Ta films, and measured the in-plane electrical transport in these films in the same temperature range. The conductive filaments in Ta₂O₅-based memristive devices show the same transport mechanisms as those observed in the TaO_x thin films with $x \sim 1$ [1].

A deeper look into the structure of the TaO_x films reveals the presence of Ta clusters in the TaO_x films. Besides that, the TaO_x films with $x \sim 1$ exhibit the same electrical transport characteristics as the metallic Ta films. Both samples share the transport mechanisms, a carrier concentration on the order of 10^{22} cm^{-3} and a positive magnetoresistance associated with weak antilocalization at $T < 30 \text{ K}$. Therefore, it is concluded that the transport in the TaO_x films with $x \sim 1$ is dominated by a percolation chain of Ta clusters [2].

These results strongly support the existence of a metallic Ta conductive filament in Ta₂O₅-based memristive devices.

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Design of nanoSERS platforms for biosensing

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Surface Enhanced Raman Spectroscopy (SERS) is a highly sensitive analytical technique, in which substrate material and geometry are crucial for enhancement. For analytical applications in portable sensors, substrates that are easy to produce and disposable are highly desirable. Paper SERS devices exploit the inherent advantages of paper over rigid SERS substrates, such as wicking capability and flexibility. The porosity of the paper was found to play a determinant role in the nanoparticle distribution along the paper fibres, most of the nanoparticles being retained at the illuminated surface of the office paper substrate. A limit of detection for rhodamine-6G as low as 11.4 ± 0.2 pg could be achieved, with an analytical enhancement factor of $\approx 10^7$ for this specific analyte.[1] Moreover, functionalising the paper with polyelectrolytes such as poly(sodium 4-styrenesulfonate) (PSS) opens the possibility to produce multifunctional analytical paper platforms. Other applications involve SERS-based immunoassays based on bioconjugates of polyclonal antibodies and anisotropic gold nanoparticles (AuNSs) functionalised with a Raman reporter, 4-mercaptobenzoic acid (MBA). These bioconjugates, once loaded with the antigen analyte, can react in a sandwich format with the same antibodies immobilised on a surface. Agarose gel electrophoresis was instrumental in determining the appropriate amounts of the MBA and antibody to AuNSs, in order to fully cover the AuNS surface. Thus, these bioconjugates provide a proof-of-concept for a SERS-based immunoassay with easy adaptation to a microfluidics platform.[2]

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Crystalline silicon nanoparticles for new (opto)electronic applications

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Crystalline silicon nanoparticles (Si-NPs) are promising eco-friendly nanomaterials for (opto)electronic and biological applications owing to their interesting size-tunable physical properties. Their large surface-to-volume ratio makes them highly sensitive to surface effects, which strongly affects their properties. Using experimental and theoretical methods, we have been studying surface- and low-dimensional-related issues on Si-NPs synthesized with an industrially-scalable plasma method. For instance, we linked the surface oxidation evolution with the appearance of compressive strain in the NPs crystalline core [1,2] and the effect of the oxide shell on the light emission origin and its dependence on NP size (Fig. 1) [3]. We have also studied the role of surface-related sub band gap states on the recombination of photo-generated charge carriers [3]. Moreover, we have been studying electron-phonon interactions under intense illumination [4], due to the inefficient photo-charge diffusion in our Si-NP systems [5].

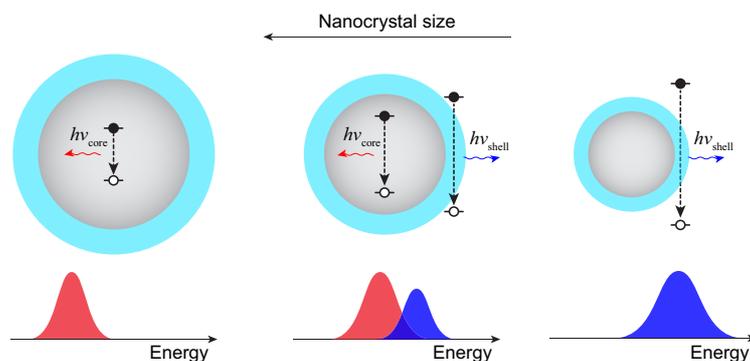


Fig. 1. Size-dependence of the origin of light emission in surface-oxidized Si-NPs.

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Cellulose Photonic Circular Polarized Light Detectors

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Cellulose Nanocrystals (CNC) when processed the right way upon drying self-assemble into photonic chiral nematic films that selectively reflect left-handed and transmit right-handed circular polarized light (CPL). Our group focuses on the use of paper in microelectronic devices. With this work we show how to use CNC films and membranes in transistors and light sensors, exploiting their dielectric and photonic character. The CNCs are obtained through acid-hydrolysis from microcrystalline cellulose and concentrated in water until around 3 wt%. Photonic films are fabricated through drop-casting CNC suspensions onto Glass/ITO and consequent self-assembly. The dry films can then be further modified with functional thin-films through physical vapor deposition. The used devices for sensing consist of an IGZO semiconductor with aluminum electrodes. IGZO is a light sensitive metal oxide, which responds to the photonic properties of CNC films with a change in resistivity. The CNCs are employed as gate dielectrics in sputtered amorphous indium–gallium–zinc oxide (a-IGZO) transistors. The obtained devices operate in depletion mode at low voltages (<2 V) with On–Off ratios of up to 7 orders of magnitude, subthreshold swings around 80 mV dec^{-1} , and saturation mobilities up to 9 cm^2 V^{-1} s^{-1} . Combining the photonic character of the CNC films with the light sensitivity of a-IGZO, the devices are capable of discrimination between left- and right CPL signals in the blue region. These types of devices can find application in photonics, sensing with CPL but also imaging.

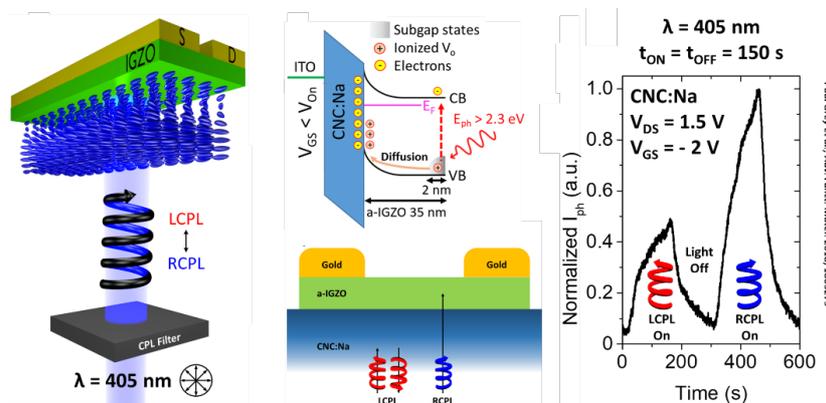


Fig. 1. Device representation and mechanism of CPL sensing with $\lambda=405$ nm.

Graphene foams and membranes for electromechanical sensing

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With the uprising of the internet-of-things, a crave for both cheap and high-performance new generation sensors emerged to feed this new paradigm with data. Graphene is demonstrating its potential as a sensing platform in areas as distinct as photodetection, bio-sensing and mechanical sensing, among others. In the case of graphene electro-mechanical sensors, piezoresistive sensing has been one of the most studied mechanisms in both pristine graphene films, single/multi-layered, and reduced graphene oxide foams and composites. In our group, we explore both CVD graphene and Laser-Induced Graphene (LIG) as sensing platforms, devising different mechanical sensors. LIG sensors were patterned as strain gauges in polyimide films and used as sensitive and low-cost piezoresistive arterial waveform sensors [1]. Few layered CVD graphene was used to produce a broadband capacitive microphone through a new transfer method which allowed to achieve the best aspect ratio (lateral dimension over number of layers) for graphene membranes in literature.

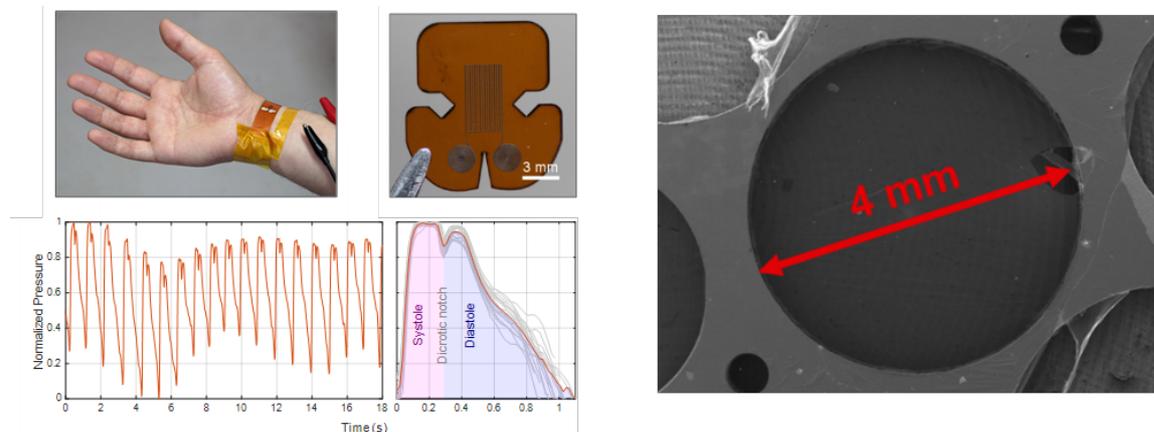


Fig. 1 Left: LIG strain gauges used in the measurement of the arterial pressure waveform and an example of data collected. Right: few-layered 4 mm wide graphene membrane.

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Magnetic bioactive glass-based 3D systems for bone cancer therapy and regeneration

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The treatment of malignant bone disease and the regeneration of large bone defects still represent a significant clinical challenge [1]. Therefore, a polymeric scaffold for bone regeneration that simultaneously kills residual tumor cells is of much benefit. After tumor extirpation, the local recurrence of the tumor cells is a major concern which requires further treatment as well. Magnetic hyperthermia has emerged as a potential cancer treatment option, since it is considered an effective treatment without adverse side effects [2]. Mesoporous bioactive glasses (MBGs) have gained much attention because they are highly bioactive and their dissolution products affect osteoblast cell gene expression and have potential effect on angiogenesis and neovascularisation, which promotes bone healing. In this work a new concept for the treatment of bone disease and simultaneous regeneration of bone defects is proposed: a polymeric scaffold (polyvinylpyrrolidone) produced by electrospinning containing MBG 80S15 and superparamagnetic iron oxide nanoparticles (SPIONs). Such composite should be able to act as a scaffold for new healthy regeneration and simultaneously kill residual tumor cells through magnetic hyperthermia. This new concept has the potential to overcome the harmful of conventional cancer therapies such as chemotherapy and radiotherapy.

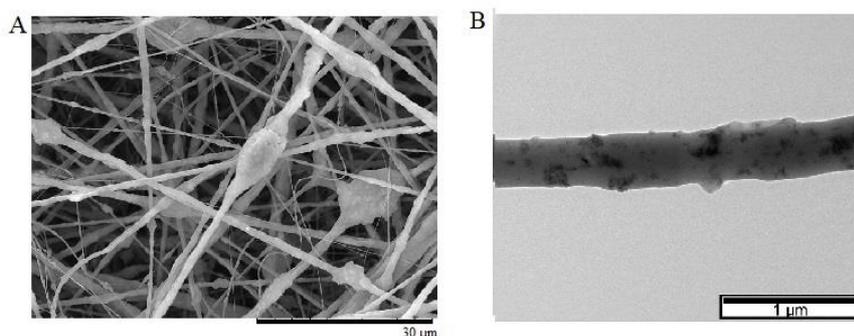


Fig. 1. SEM image of PVP/MBG 80S15 composite (A) and TEM image of PVP/SPIONs (B).

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Investigation of ferroic nanostructures for energy and environment

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We have been working on the development of environmental friendly ferroic nanostructures for energy harvesting based on the principles of piezoelectricity, magnetoelectric coupling, photocatalysis and pyroelectricity. Ferroic structures of perovskites, electroactive polymers, Aurivillius layers in thin film and single crystal forms are being explored to find coupling between various functionalities.

In order to avoid environmentally hazardous fluorinated coolants employed in compression-expansion based refrigeration, electrocaloric effect (ECE) is being under intense investigations since the devices can be scaled down to accessible sizes (on-chip). ECE is a cost-effective process and requires polar structures with strong polarization switching so that the effects are stronger near ferroelectric-paraelectric phase transition temperatures. We have been working on lead-free ferroelectrics with morphotropic phase boundary, having phase transitions near room temperature, to achieve higher changes in adiabatic temperature (ΔT) and isothermal entropy (ΔS).

We also present studies on Aurivillius ferroelectrics which can be alternatives to titania based nanostructures, to degrade environmentally hazardous gases that can cause smog. In our study, Bismuth layered oxides exhibited a strong photo-catalytic activity (PCA) in liquid phase as well as gas-solid phase experiments to degrade organic pollutants as well as toxic NO_x .

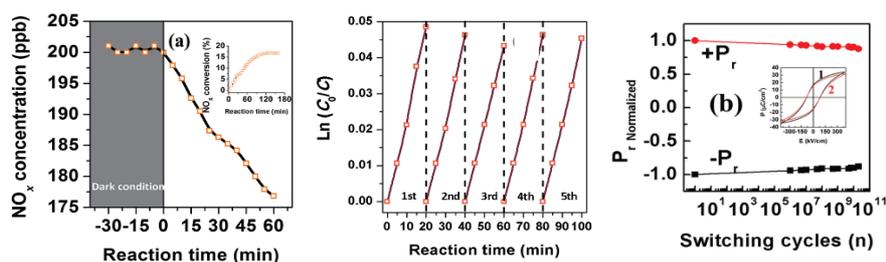


Fig. 1 (a) PCA abatement of NO_x gas by a 3-layered Aurivillius ferroelectric. (b) Fatigue resistance of 5-layered Aurivillius thin film up to 10^{10} cycles, 1 and 2 represent switching before and after fatigue.

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Solution Processed Halide Perovskite Thin Film Transistor

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Organolead halide perovskites have drawn significant attention from the scientific community as one of the most attractive materials in optoelectronics, especially in the field of photovoltaics. In this study, we focus on using halide perovskites in thin film transistors (TFTs). Halide perovskites have high solution processability and excellent carrier transport characteristics, in particular for holes. The present work aims to fill a gap on oxide-based technology. It concerns the process of using high-stable and reliable p-type oxide-based devices to target CMOS technology (complementary metal-oxide-semiconductor). We report on a solution processed high performance TFT based on methylammonium lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) perovskite semiconductor films, which shows promise for devices that can be simple to manufacture with high reliability, reproducibility and excellent stability in atmospheric conditions. The introduction of diethylsulfide (DES) in the perovskite precursor paves a way to achieve a highly stable perovskite semiconductor film. The TFT shows a stable p-type behavior when operated at low voltages (≤ -3 V), has a current modulation $> 10^4$, an almost neglected hysteresis and average saturation mobility $28.5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. This is the highest value till now reported in the literature. In addition, we demonstrate that perovskite TFTs can be fabricated at temperatures as low as 150°C on flexible substrates with a saturation mobility of $\sim 22.7 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. The high performance TFT with excellent stability made via low temperature solution processed technique opens a new pathway for the perovskites as a promising candidate for the next generation of p-type transistors for a plethora of low-cost electronics applications.

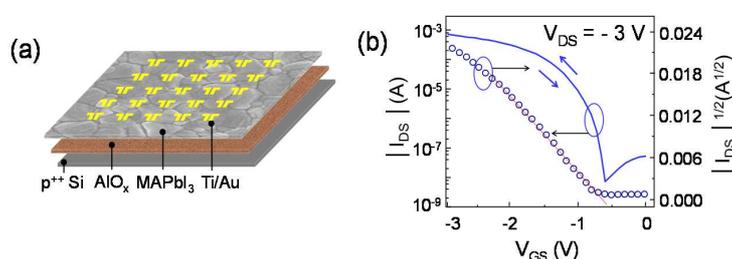


Fig. 1. (a) Schematic of TFT showing the Ti/Au Drain Source metal contacts, deposited via shadow masks; the MAPbI₃ as semiconducting channel. Transfer characteristics (module of I_{DS} and $I_{DS}^{1/2}$ vs V_{GS} at constant $V_{DS} = -3$ V) of MAPbI₃-DES based TFT.

DEVELOPING BIOMATERIALS & CERAMICS FOR INDUSTRIAL APPLICATIONS

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DentalBlast project

Dental implants have been used quite frequently in dentistry. However, about one in five patients develop peri-implantitis after five years of implantation. This infection causes the removal of the implant and is currently the main cause of this nonconservative treatment, which must be avoided. Given this drawback, the use of a bioactive material with antibacterial activity, in the surface of the implants, has been seen as an innovative solution. Within the biomaterial family, it was reported by Hench et al. some particular glasses of the $\text{SiO}_2\text{-P}_2\text{O}_5\text{-CaO-Na}_2\text{O}$ system which forms a stable and adherent bond with the natural bone and high bioactive potential. One of those is the 45S5 Bioglass[®]. One of the main advantages of these biomaterials is the possibility of change, easily, its composition being possible to increase its bioactivity, stimulate osteogenesis and angiogenesis effects and also add other properties such as the antibacterial. For example, it is already known that silver has enormous potential for antimicrobial activity. Therefore, the introduction in the bioglass network of silver ions can promote an antibacterial effect, without changing the glass bioactivity.

CerWave project

Portuguese energy dependence on fossil resources exceeds 85%. The ceramic industry is a highly consuming thermal energy, required in the drying and firing process. The growing competitiveness, needs and opportunities, boost in the search of alternative and more energy-efficient technologies. A new method that uses microwave radiation for the porcelain firing is presented. The specificities of highest volumetric heating, centered in the material as a direct result of the electromagnetic radiation absorption, allow the prediction of shorter processing times, speeding up the processes, with a possible reduction of the sintering temperature and with less harmful gases emissions.

Design of optimized photonic microstructures coupled with luminescent down-shifting for high-efficient, flexible and stable perovskite solar cells

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Recently, perovskite solar cells (PSCs) have shown outstanding capability to play vital roles in overcoming global energy crisis, demonstrating the fastest growing PV efficiency in a few years. Despite impressively high efficiencies (>23%), PSCs face several challenges such as poor stability due to fast degradation upon UV exposure, water and moisture penetration, etc [1].

In this context, optical solutions are promising avenues for improving not only the PSCs efficiency, by allowing the use of thinner absorber layers, but also their market applicability by enabling higher device flexibility and improve stability. Here, a solution is proposed that can minimize the UV degradation effect while boosting the cells' generated photocurrent, by making use of combined light-trapping (LT) and luminescent down-shifting (LDSs) effects capable of pronouncedly improving the photocurrent, enabling the reduction of the cell thickness to half, and changing the harmful UV radiation to higher wavelengths that can be effectively “trapped” in the solar cell.[1-3]

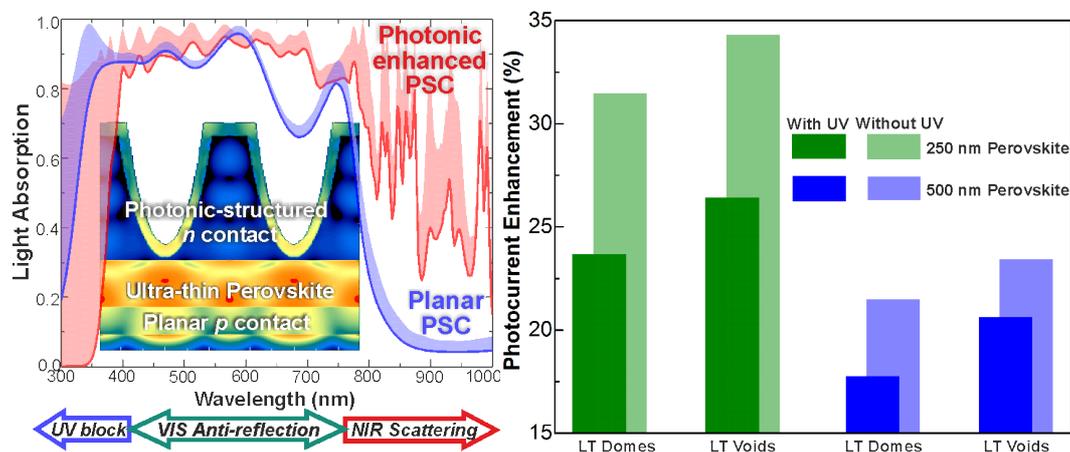


Fig. 1. Left - simulated light absorption profile for the best LT case in Perovskite solar cells. Right - photocurrent enhancements attained with the two types of optimized LT structures based on TiO₂ voids or domes arrays, relative to the planar reference cells.

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Optical fiber sensor networks for in situ lithium-ion batteries monitoring

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According with the Paris agreement (COP21), as well as the EU 2030 targets, there is a need for significant reductions in CO₂ and greenhouse gas emissions in a short time span. Electric batteries, such as lithium-ion batteries (LIBs), are currently seen as important technological enablers to drive the transition towards a decarbonised society. The sensing of characteristic parameters in LIBs, such as temperature and strain variations are fundamental issues to ensure that they operate in safe conditions. Typically, they are externally monitored through electronic sensing devices, such as thermocouples, micro-electro-mechanical systems, and pyrometers. However, in addition to low resolution and accuracy, these sensors are not suitable to be embedded, due to the electrochemical environment of the battery. Alternative solutions, with higher precision, multipoint and multiplexing capabilities, and easily integrated in LIBs with low invasiveness are the optical fiber sensors (OFS) (see Fig.1). OFS embedded in LIBs will contribute to a better knowledge of their internal and external LIB performance, improving safety and optimize the design of the next generation of LIBs.

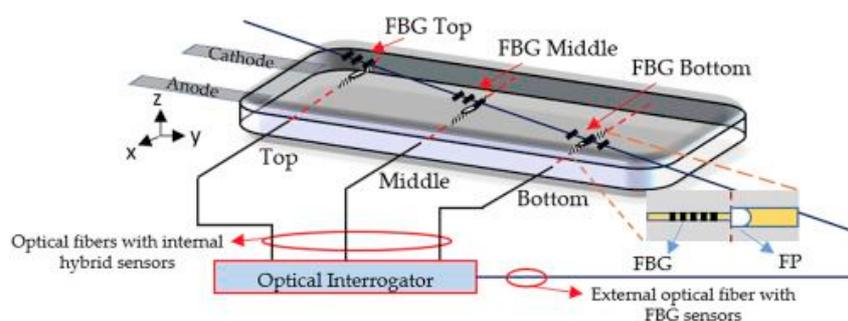


Fig. 1. Intergration of optical fiber sensors in Li-ion batteries to monitor characteristic parameters.

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Type of Presentation: Poster

Nanoscale Data Storage by Probe Induced Charge Injection Method

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The increasing demand for miniaturization in microelectronics has led to an upsurge interest in developing nanoscale electrical characterization as a part of the effort to enhancing nanoelectronics. As the size of electronic device is scaled down towards the nanometre-dimensions, atomic force microscope (AFM) can be used as a technique of choice to study the influence of controlled charge injection phenomenon into the materials by electrically biased AFM probe at the time of scanning. Though, the controlling operation with knowledge in localized charge-transport dynamics of nanometer-sized device remains both critical and challenging.

In that context, we report on the study of direct visualization of charge propagation through the organic/inorganic nanostructures via nano-contact probe induced charge (both positive and negative) injection (PiCi) method through AFM. The experimental works open a way for ‘writing-reading’ of memory bits using electrical bias towards the development of next generation charge trapping data storage devices with establish of smallest bits memory cells. During contact mode, external electrical bias has been applied through AFM probe which locally injects the charge (or extracts the charge depending on the polarity of applying voltage) into the nanostructures. The core idea of this device is charge patterning through charge trapping mechanism, which is visualized further by the subsequent electrical mapping. In pursuit of this PiCi mechanism towards the ‘writing’ ability on nanostructure surface, we performed the electrical mapping of that region with a larger area, which can be explained as a ‘read-out’ image. Furthermore, to acquire the smallest ‘bit’ of stored information, we deployed the AFM probe on a single point of device layer and write–read–erase–read cycles were performed with write/erase pulses using optimised negative and positive voltages, respectively, for different pulse duration.

Work has been projected to target the next generation electrical-nanoimprinting nanostructure data-sheet based on PiCi mechanism.

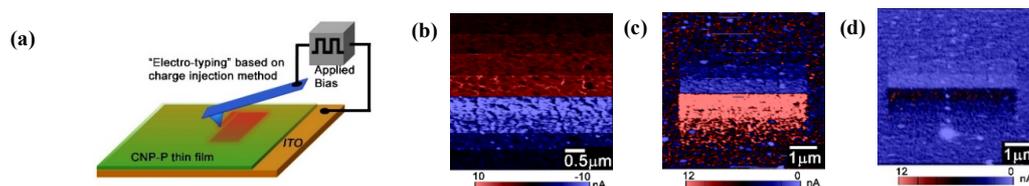


Fig. 1. (a) Schematic of charge injection through AFM probe. (b) Visualization of current mapping during charge injection with different bias voltage (from ± 1 to ± 7 V). Visualization of current mapping after charge injection using (c) +5V and (d) +1V bias voltage.

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Development and optimization of optical fibre sensors by a femtosecond laser

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Fibre optic sensors (FOS) are devices capable of sensing several physical and chemical parameters and, due to its intrinsic advantages (low weight, electromagnetic immunity, low transmission loss, etc), they can be applied in different areas: ranging from civil engineering to biomedical areas. The most used types of FOS are: fibre Bragg gratings (FBGs), interferometric configurations (for example, Fabry-Pérot cavities) and based on optical power intensity variation. Since these sensors are intended to be used either in severe and/or delicate environments (for example, explosive environments and medical exams, respectively), its manufacturing have to be customized in order to optimize the final product, guaranteeing feasibility and reliability.

A 6-axis platform based on a femtosecond laser was implemented (Fig. 1 (a)), which allows the user to inscribe and/or manufacture any optical fibre sensor, as well as waveguides. FBGs and FPIs can be inscribe by 3 different methods: point-by-point, line-by-line and plane-by-plane. Parallel to this 6-axis platform, a phase-mask (PM) setup was mounted to inscribe FBGs in any type of fibre optic.

Thermal stability tests were conducted in a customized micro-oven to assess the FBGs' lifetime, which revealed a decrease in the maximum optical power peak and a wavelength blue shift with increasing temperature. Also, a novel magnetic field sensor was developed based on a FPI cavity between a silica fibre and a fuse effect damaged polymeric fibre (Fig. 1 (b) and (c)), revealing a sensibility up-to 50 pm/mT in the region of 0 to 40 mT.

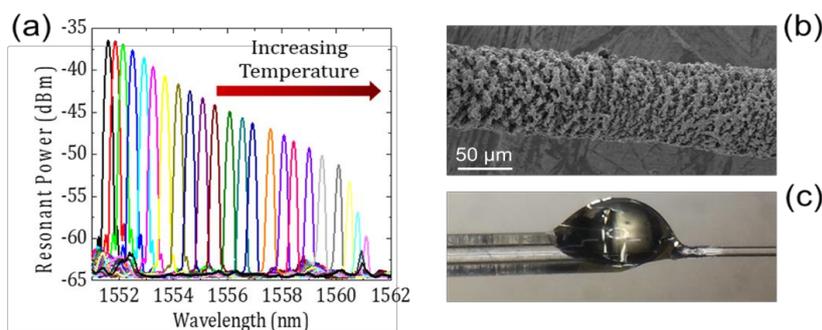


Fig. 1. (a) Thermal calibration of a FBG; (b) SEM image of a polymeric fibre core damaged by fuse effect; (c) Microscope image of the developed magnetic field sensor.

Structurally colored bio-inspired sustainable materials from nanocellulose composites

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The beautiful iridescent colors that can be observed in evaporated self-assembly cellulose nanocrystal (CNC) films, arising from their liquid crystalline phase, has lately inspired several scientists. In addition to this property and their selective reflection of left-handed circularly polarised (LCP) light, one can also find some micrometer-gaps. These gaps, which can be found perpendicular to the cross-section of a CNCs' film, can be filled with a nematic low molecular weight liquid crystal and give rise to a system that reflects both right- and left-handed circularly polarized light (RCP and LCP) as can be seen in Figure 1. In this system, the nematic layer acts as a half-wave retardation plate, as observed in certain beetles' exocuticle (*Chrysina resplendens* (Boucard, 1875)), and the system is reversibly tuned by variation of either electric field or temperature. The use of iridescent CNC films with diverse optical responses combined with different liquid crystals can give rise to complex systems with enhanced optical responses. Inspired by this work some interesting cellulose composite systems are being developed.

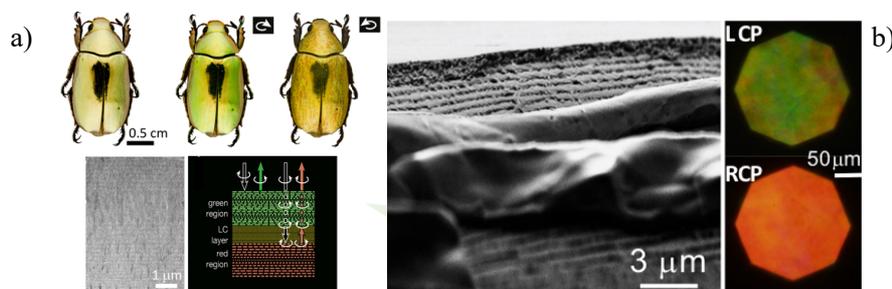


Fig. 1. a) *Chrysina resplendens* beetle observed at normal, left-handed and right-handed polarized light bottom TEM-image of the beetles exocuticle¹. b) SEM image of a cross-section of the bio-inspired CNC film with a micro-gap filled with 4CB, where top and bottom cholesteric domains have different pitch sizes (left). Optical images of left- and right-handed circularly polarized light reflectance of a CNC/5CB composite system (right).²

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