i3N INSTITUTE FOR NANOSTRUCTURES, NANOMODELLING AND NANOFABRICATION

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Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa (FCT-UNL), Main Host
Universidade de Aveiro (UA)
Universidade do Minho (UM Institution)

VI ANNUAL MEETING – 24/25FEV17

LISBOA

ACKNOWLEDGEMENTS

VI Annual Meeting i3N, Lisboa 2017

24-25 February 2017

Cofinanciado por:

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i3N

INSTITUTE FOR NANOSTRUCTURES, NANOMODELLING AND NANOFABRICATION

RESEARCH, INNOVATION AND ENGINEERING APPLICATIONS

Book of Abstracts

VI Annual Meeting i3N, Lisboa 2017

24-25 February 2017

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WELCOME TO UNL

Nanosciences and Nanotechnology in strong relation with Advanced Materials, are key elements for today's society and at i3N we have now a double responsibility, because we have achieved the highest mark of "EXCEPTIONAL" from the last evaluation done by FCT-MCTES, and now we will be evaluated again, during this year, so it is quite important to keep the previous mark, placing again i3N as the leading Portuguese research unit in the areas of Nanotechnology and Advanced Materials.

At i3N we believe that the combined strengths of a collaborative team is by far, orders of magnitude greater than the sum of the individuals. In a multidisciplinary field such as Nanotechnology this is even stronger.

i3N is organized into 9 research groups with a strong interaction under 3 main thematic lines:

- Micro/Nano Integration into Demonstrator Systems
- Theoretical and Computational Studies on Materials and Devices/Systems behaviour
- Advanced Micro/Nano Materials and Technologies

This year we would like to thank again all the authors and a special thank to Dr. Manuel Bibes from CNRS/THALES/University Paris Sud, from the laboratory of Prof. Albert Fert Nobel Prize in Physics 2007.

And keeping our main roots as it was said by Ricardo Reis:

"Para ser grande, sê inteiro: nada

Teu exagera ou exclui.

Sê todo em cada coisa. Põe quanto és

No mínimo que fazes.

Assim em cada lago a lua toda

Brilha, porque alta vive."

Enjoy the meeting and your time in Lisbon.

Elvira Fortunato
I3N Director

PROGRAMME

Friday, 24 February 2017

11h00-11h45 Registration / Posters (Rectorate Hall)

11h45-12h00 Opening Ceremony (Auditorium B)

12h00-14h00 Lunch and Poster Session (Rectorate Hall)

14h00-14h50 Invited Plenary:

Dr. Manuel Bibes, CNRS Research Director) Oxide Heterostructures for Electronics and Spintronics (Auditorium B)

14h50-16h30 Group presentations – 1st (Each presentation will be 20 minutes)

-Materials for Electronics, Optoelectronics and Nanotechnologies, Prof. Dr. Rodrigo Martins, CENIMAT-FCT/UNL
-Soft and biofunctional materials group, Prof. Dr. João Paulo Borges, CENIMAT – FCT/UNL
-Structural Materials, Prof. Dr. Francisco Braz Fernandes, CENIMAT – FCT/UNL
-IPC through 2016 – outputs and new frontiers, Julio C. Viana, António Pontes

16h30-17h00 Coffee Break and Poster Session (Rectorate Hall)

17h00-18h20 Group presentations – 2nd (Auditorium B) (Each presentation will be 20 minutes):

-Semiconductors Physics, Prof. Dr. Armando Neves, UAveiro
-Theoretical and Computational Physics, Prof. Dr. Ricardo Dias, UAveiro
-Novel Materials and Bio-systems, Prof. Dr. Manuel Almeida Valente, UAveiro
-Optics and Optoelectronics, Prof. Dr. João de Lemos Pinto, UAveiro

18h20-18h45 Keynote I (Invited)

18h45-19h10 Keynote II (Invited)

20h00 Dinner Rectorate Hall

Saturday, 25 February 2017

09h00-10h30 General Meeting (Auditorium B)

10h30-11h00 Coffee Break (Rectorate Hall)

11h00 Closing (Auditorium B)

GENERAL INFORMATION

Conference Venue

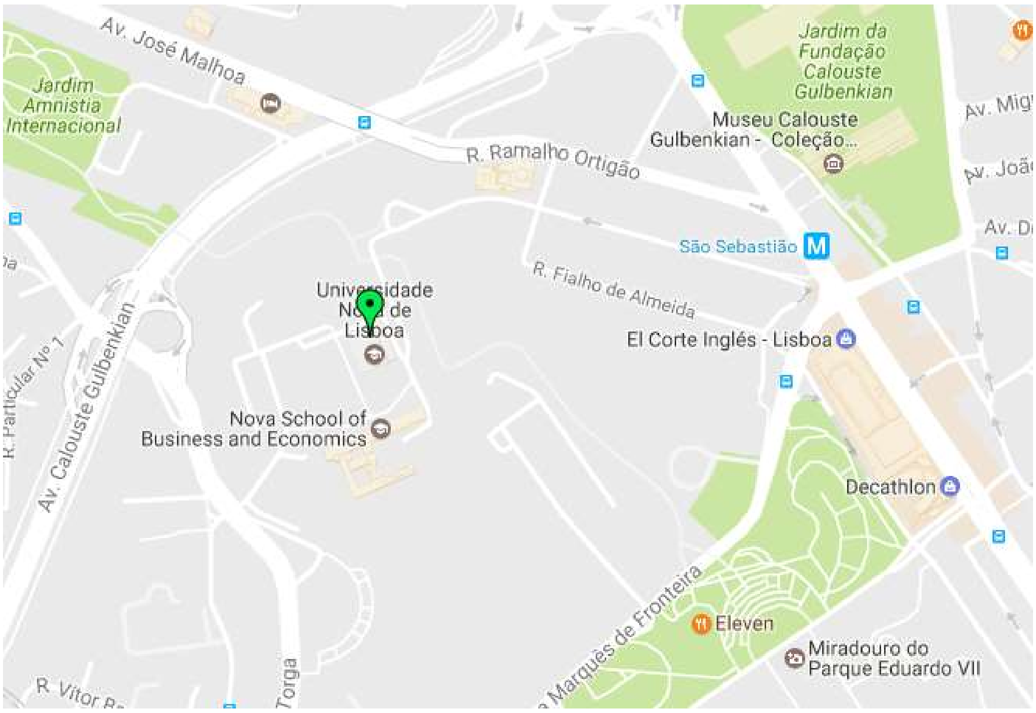
The "VI Annual Meeting i3N" will be held in NOVA's Rectorate on 24-25th February 2017.

Address

Rectorate
Universidade Nova de Lisboa

Campus de Campolide

1099-085 Lisboa



GENERAL INFORMATION

About Lisbon

Lisbon is one of the oldest cities in the world, and the oldest in Western Europe, predating other modern European capitals such as London, Paris and Rome. Located in the western Iberian Peninsula on the Atlantic Ocean and the River Tagus where the westernmost areas of its metro area is the westernmost point of Continental Europe.

Lisbon Is the capital and the largest city of Portugal, with a population of 552,700 within its administrative limits in an area of 100.05 km². Its urban area extends beyond the city's administrative limits with a population of around 2.7 million people, being the 11th-most populous urban area in the European Union. About 2.8 million people live in the Lisbon Metropolitan Area (which represents approximately 27% of the country's population). Recognised as a global city because of its importance in finance, commerce, media, entertainment, arts, international trade, education and tourism. The city is the 7th-most-visited city in Southern Europe.

Lisbon is a historical city where old customs and ancient history intermix with cultural entertainment and hi-tech innovation. Lisbon is the right place to listen to Fado and discover one if the thousands of ways to cook/eat the beloved *bacalhau*. Lisbon is famous for its hospitality and the family-like way it welcomes visitors.

http://www.cm-lisboa.pt/en/visit/the-city

GENERAL INFORMATION

Faculty of Sciences and Technology (FCT NOVA)

The Faculty of Sciences and Technology (FCT NOVA), Campus of Caparica is one of the most prestigious Portuguese engineering and science public schools and it is engaged in extensive research activity developed in 16 research centres involving 1600 PhD and Master's students of the total enrolment of 7800.

With a total of 550 academic staff (90% holding a Ph.D) and 180 non-academic staff, FCT NOVA is organized in 14 departments and 14 support services.

FCT NOVA partners with foreign universities such as the Massachusetts Institute of Technology (MIT), the University of Carnegie Mellon and the University of Texas at Austin to offer some of its advanced study programs. The entrepreneurial drive of the students and graduates of FCT NOVA has led to many successful spin-offs that transfer knowledge to the market and help create value and social impact.

FACULDADE DE CIÊNCIAS E TECNOLOGIA UNIVERSIDADE NOVA DE LISBOA

http://www.fct.unl.pt/en

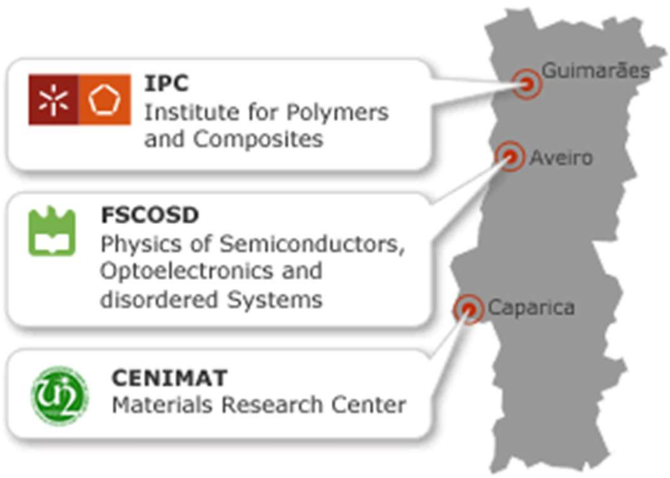
i3N

I3N, the Institute of Nanostructures, Nanomodelling and Nanofabrication was granted the status of Associated Laboratory on November 16th, 2006, by the Portuguese minister of Science, Technology and Higher Education, José Mariano Gago.

I3N is one of the major portuguese institutions in the area of nanosciences and nanotechnologies.

I3N is a partnership between three leading research units in fundamental and applied science: IPC (Institute for Polymers and Composites, hosted by University of Minho), CENIMAT (Materials Research Center, hosted by the New University of Lisbon) and FSCOSD (Physics of Semiconductors, Optoelectronics and disordered Systems, hosted by the University of Aveiro). Over one hundred researchers are currently involved in multidisciplinary fundamental and applied research projects in four broad domains:

- multi-scale modeling of materials behaviour;
- nanofabrication , micro and nano technologies;
- polymer systems with nano and microcontrolled structures;
- physical characterization of nanostructures.



http://www.i3n.org/

INVITED TALK

Manuel Bibes (CNRS Research Director at the CNRS/Thales laboratory in Palaiseau, France**)**

Manuel Bibes (Sainte-Foy-la-Grande, France, 1976) is a CNRS Research Director at the CNRS/Thales laboratory in Palaiseau, France. After graduating as an Engineer in Materials Physics (INSA Toulouse, 1998), he obtained a double PhD degree in France and Spain with a thesis on manganite interfaces supervised by J. Fontcuberta (ICMAB Barcelona, 2001). Following two years of postdoctoral work on oxide spintronics with A. Fert in Orsay he became a CNRS Researcher in 2003. Bibes then pioneered research lines on multiferroics and oxide-based spin-filter junctions and in 2009, he led the discovery of giant electroresistance in ferroelectric tunnel junctions and patented their use as ferroelectric memristors. He also explored novel routes for the electrical control of magnetism and spin transport in hybrid oxide-metal architectures. Bibes is the recipient of the 2013 EU40 Materials Prize of the E-MRS, an APS Fellow, and the laureate of a European Research Council grant to design novel states of matter through electronic correlations. He has coauthored more than 150 articles in international journals totalizing around 10000 citations, filed 7 patents and given over 140 invited talks at conferences and research institutes.

https://oxitronics.wordpress.com/people/manuel-bibes/

GROUP PRESENTATIONS

Prof. Dr. Rodrigo Martins

Materials for Electronics, Optoelectronics and Nanotechnologies
CENIMAT

Soft and Biofunctional Materials Group
CENIMAT

Prof. Dr. João Paulo Borges

Prof. Dr. Francisco Braz Fernandes

Structural Materials
CENIMAT

Institute for Polymers and Composites
MINHO

Prof. Dr. Júlio Viana
Prof. Dr. António Pontes

Prof. Dr. Armando Neves

Semiconductors Physics
UAveiro

Theoretical and Computacional Physics
UAveiro

Prof. Dr. Ricardo Dias

Prof. Dr. Manuel Valente
UAveiro

Novel Materials and Bio-Systems
UAveiro

Optics and Optoelectronics
UAveiro

Prof. Dr. João Lemos Pinto

Materials for Electronics, Optoelectronics and Nanotechnologies (MEON)

R. Martins
Departament of Materials Science/i3N, FCT-UNL, Campus de Caparica, 2829-516 Caparica, Portugal

The MEON group is centering is activity in the key areas of advanced functional materials for electronics, energy, health and security applications, emphasizing the role that circular economy and substitution as for the strategy of the future, globally. To do so we exploit the multifunctionalities of the materials at a nano and micro scales going from low cost and reliable processes (physical, chemical and mixed methods) followed by a proper heat treatment, to devices and systems, integrated in low cost platforms, back up by proper design, modeling and test/validation operations. Here the target of our activity concerns transparent and flexible electronics; to develop paper electronics, as new areas of societal impacts, where nanotechnologies and microelectronics concepts must be fully aggregated novel electrochromic and thermoelectric materials; solar cells based in novel photonics concepts; thin film transistors; CMOS; nanogenerators based in novel piezoelectric concepts; ring oscillators; power controllers; logic gate circuits; amplifiers; memories, sensors, among others, combined or not with organic materials, aiming to develop a new generation of smart systems away from silicon. The materials and devices developed targets mainly the field of low cost and disposable devices/systems of great relevancy for our future such as intelligent packaging, smart labels for food and pharmaceutics industry; full disposable active and passive bio-detection platforms for a broad range of applications, all full recyclable. microfluidic platform for a broad range of analysis, as DNA via colorimetric methods based on gold nanoparticles plasmonics, using different configurations and substrates, as paper.

SOFT AND BIOFUNCTIONAL MATERIALS GROUP AT A GLANCE

João Paulo Borges

SBMG-CENIMAT/i3N, FCT-NOVA, Portugal

The Soft and Biofunctional Materials Group is much involved in the study of polymeric and mesomorphic materials, with focus on cellulose- and chitin/chitosan-based systems. The structure of those materials as well as their dynamics at the mesoscopic scales determines their physical properties which have been explored to develop new biomimetic materials. Different polymeric systems studied in the group have potential applications in electrooptical devices, electrorheological fluids and product development and biomedicine.

The techniques we used include light scattering, microscopy, rheology (Rheo), nuclear magnetic resonance (NMR), Rheo-NMR, magnetic resonance imaging (MRI), electrospinning and microfluidics.

Structural Materials Research Group - Overview

F.M. Braz Fernandes

SM-CENIMAT/i3N, FCT-NOVA, Portugal

The Structural Materials RG has been focusing its activity on the production of nanostructured materials (metals, ceramics and composites) as well as on techniques of micro and nano-characterization. Taking profit of previous experience, the members of the RG have been applying for projects for synchrotron radiation beam time (ESRF, at Grenoble and PETRA III, at Hamburg), aiming at micro/nano-characterization. The following topics will be focussed upon:

TL1 Theoretical and Computational Studies on Materials and Devices/Systems Behaviour
- development of parallel-computing image processing techniques applied to micro and nanotomography.
- computer modelling and simulation of functionally graded composites' microstructure during fabrication by centrifugal casting.
- modelling of mechanical behaviour boundaries for biomimetic chitin/chitosan films for biomedic applications (in collaboration with J.P. Borges).

TL2 Advanced Micro/Nano Materials and Technologies
- functionally graded alloys and composites through Severe Plastic Deformation, using ECAP and FSP methods, namely in shape memory alloys (SMAs);
-development of functionally graded syntactic and auxetic foams for biomedical and structural applications (in collaboration with J.P. Borges);
- synthesis and characterization of nanostructured glasses and glass-ceramics for application in photonics.

TL3 Micro/Nano Integration into Demonstrator Systems
- applications to civil engineering, shape morphing using polymer based matrices and biomedical (endodontics and orthodontics) of SMAs;

SP4 Structural characterization
- micro/nano characterization through the application of synchrotron radiation
- micro/nano characterization of long term corrosion using archeological samples and of historic metals and metallurgical related materials;
- laboratory (thermal, mechanical and structural characterization techniqes) and synchrotron radiation based techniques applied to cultural heritage materials (ceramic and lithologic origin) and to SMA thermomechanical processing / welding.

IPC through 2016 – Outputs and New Frontiers

J.C. Viana, A.J. Pontes

IPC-Institute for Polymers and Composites/i3N, University of Minho, Campus de Azurém, 4800-058 Guimarães. Portugal

The research activities at IPC/i3N – Institute for Polymers and Composites during 2016 were characterised by the consolidtion of the activities of the strategic plan and by the initiation of new projects (after closure of all funded national projects by FCT and QREN and European projects in 2015). The main outputs of IPC in 2016 were:

- 13 new R&D projects started, in a total of captured funding of 3,72 M€
- 63 articles published in international jornals, 7 full articles in international conferences, and 5 chapters in international books, in a total of 75 publications, corresponding to an average of 2,8 publications per integrated PhD.
- 5 PhD and 37 MSc concluded
- 3 national and 1 international conferences organised

In this preentation will be detailed the new projects that started at IPC/UMinho in 2016:

- *TSSiPRO - Technologies for sustainable and smart innovative products* (NORTE-01-0145-FEDER-000015 – TSSiPRO). The project will investigate sustainable and smart innovative technologies and systems based on polymers and textiles, integrating ICT (embedded electronic systems) and design and eco-design tools. Entities: UMINHO (**IPC**, 2C2T, Algoritmi, Lab2PT) (total/IPC: 3.686,8/1.622,2 k€) (may 2016 - apr 2019)
- *IAMAT - Introduction of advanced materials technologies into new product development for the mobility industries* (MITP-TB/PFM/0005/2013). Goal: to develop an integrated framework for product development evaluation that can exploit the potential of the use of advanced materials, manufacturing technologies and structures in the aerospace industry. Entities: **FEUP**, UMinho (IPC, Algoritmi), IST, Embraer, Optimal, MIT (total/IPC: 979,9/229,9 k€) (jan 2016 - dec 2018)
- *FIBR3D - Additive Manufacturing-based hybrid process for long or continuous fibre reinforced thermoplastic matrix composites* (Compete-016414). Main goal: development of a hybrid and integrated process that combines, into a single platform, additive and subtractive operations and allows CAD-to-Part productions with freeform shapes using long or continuous FRTP. Entities: **INEGI**, i3N (CENIMAT, FSCOSD, IPC), Algoritmi, LAETA, IDMEC, UNIDEMI, (total/IPC: 2.499,2/484,0 k€) (set 2016 - ago 2019)
- *MOLDPRO - Multi-scale approximations for injection moulding of plastic materials* (ref. PTDC/EMS-ENE/3362/2014). Goal: to develop stable, accurate and parallelized numerical codes for the prediction of single and two-phase flows of thermo-rheologically complex fluids using the Proper Generalized Decomposition (PGD) technique. Entities: CEFT/FEUP, IPC (total/IPC: 157,9/67,3 k€) (jul 2016 - jun 2019)
- *IMPULSE - Polymers and composites: Drivers of technological innovation and industrial competitiveness* (NORTE-08-5369-FSE-000034). Doctoral programme aiming at training the next generation of leaders for technological innovation and industrial competitiveness in polymers and composites, and at meeting the needs of the sectorial stakeholders, transfering knowledge. Entities: **IPC**, PIEP, CEIIA, CTCP, CENTI, CENTIMFE (total/IPC: 445,5/445,5 k€) (out 2016 - set 2019)

- *INNOVCAR – Innovative Car HMI* (AAC nº 07/SI/2015 - nº 002797). Goal: developing knowledge and technologies for the car of the future, namely as regards more advanced driver assistance and navigation systems and components (including topics such as safety, comfort and environment). Entities: Bosch Car Multimedia, UMinho (IPC, others) (33.390,7 k€) (Jul 2015- Jun 2018)
- *iFACTORY- New industrialization concepts* (AAC nº 07/SI/2015 - nº 002814). The project develops new manufacturing processes and systems. Entities Bosch Car Multimedia, UMinho (IPC, others) (23.407,6 k€) (Jul 2015- Jun 2018)
- *SMIT - Smart Multifunctional Integrated Tool* (ref. ANI-17735). Goal: to research and to development innovative multifunctional moulding solutions that enable the production of high added value products through the integration of materials, components and technologies. Entities: ITJ, RTJ, CENFIMFE, UMinho (IPC e Algoritmi) (total/IPC: 961,9/67,3 k€) (oct 2016 - ago 2019)
- *SMART COVER POOL & DECK - Soluções inovadoras para piscinas inteligentes, seguras e sustentáveis* (ref. ANI-17656). Goal: to develop new products for swimming pools, based on innovative solutions (transparent profile for swimming pool covers, decking profile for floor covering, supporting substructure for decking. Entities: SOPREFA, IPC, TEMA/UA, CTCP (total/IPC: 638,8/197,3 k€) (oct 2016 - set 2019)
- *CompositeStering - High Pressure Thermoplastic Composite Duct* (ref. ANI-018024). Goal: design and develop new technological approaches of production, based on an innovative product associated with the hydraulic automobile power steering system. Involved entities: MoldetipoII, Placidoroque, CDRSP, IPC, (total/IPC: 1.009,8/200,5 k€) (jun 2016 - mai 2019)
- *INTERAGE* - (ref. NORTE-01-0247-FEDER-017967) (total/IPC: 1.375,9/124,6 k€) (out 2016 - mai 2019)
- *ECO Sustainable Rail* - (ANI). Goal: to use mixed plastics waste (MP) as raw material for the production of eco-sustainable railway sleepers. Entities: EXTRUPLAS, PIEP, IPC, CVR, IP (total/IPC: 290,3/12,0 k€) (set 2016 - jun 2019)
- *Production of Electrically Conductive Thermoplastic Filament using Graphene* - (ESA). to produce electrically conductive thermoplastic filament using graphene, carbon nanotubes, and an engineering thermoplastic, for FDM application (for ESA). Entities: PIEP, IPC (total/IPC: 50,0/9,0 k€) (jan 2016 - jun 2016)
- Estudo sobre processabilidade de PET reciclado, obtido pelo processo de reciclagem mecânica (NORTE-01-0247-FEDER-008685). Entities: Ecoibéria – Reciclados Ibéricos, SA; CVR; DEP/IPC (total/IPC: 19,5/14,6 k€) (jan 2016 - dez 2016)

Semiconductor nano structures for (opto)electronics, energy and biomedical applications

Semiconductors Physics Group

Department of Physics & I3N, University of Aveir, 3810-193 Aveiro

We will report on the research activities of the Semiconductor Physics group, namely on the preparation and characterization of semiconductor micro- and nano-structured, for applications in the areas of electronics and optoelectronics, energy and bio-medical.

We report on recent developments on the study of nitride semiconductor nanostructures doped with rare earth (RE) ions, tailoring their emission for high efficiency nanodevices.

Inorganic nanoparticles, doped with RE, were produced by laser ablation in liquids, a single-step time-saving synthesis process, envisaging the production of biomarkers using up-conversion mechanisms.

Different forms of nanocarbon structures had been explored for biosensors and regenerative medicine, in this case recovering injured or permanently damaged tissues using controlled electrical stimulation.

We also developed and characterize highly efficient materials for photovoltaic applications. Most of the work was done on the physical properties and electronic structure of CZT(S,Se) and Cu(In,Ga)Se2 thin films, in order to improve the overall efficiency of the complete solar cell.

An important research area was the study on semiconductor nanoparticles, with special emphasis given to Si-NPs, focusing on several issues such as doping, optical, dielectric, and electronic transport properties, and to understand the assembling and physical processes taking place in (opto)electronic devices based on functional NPs.

New multiferroic structures for high temperature applications had been studied, as well as, the anisotropic magnetoelectric properties of differently structured piezoelectric composites or single crystals.

In the area of organic semiconductors we had developed new simple device structures of PLEDs containing active layers based on MDMO-PPV, resulting in large and efficient electroluminescence devices.

New detectors, based on scintillation materials and solid state photomultipliers, were explored for medical imaging and radiotherapy, two important fields of Medicine that use ionizing radiation. One application under development is a new concept of a preclinical Positron Emission Tomography; other a new radiation dosimeter to be used in prostate and breast brachytherapy, capable of providing real-time and in-vivo dose.

Overview of recent research carried out by the Theoretical and Computational Physics group

R.G. Dias*, M.A.S. Barroso, G. Baxter, J.P. Coutinho, R.F. Costa, S. Dorogovtsev, A.L. Ferreira, A. Goltsev, J.F.F. Mendes, J.G. Oliveira, G. Timar, V. Torres, S. Yoon

Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal

**rdias@ua.pt*

The research carried out by the Theoretical and Computational Physics (TCP) group is divided into 4 research lines: Ab-Initio Modeling of Condensed Matter; Complex Networks systems; Molecular Simulation; Quantum Transport.

The members of Ab-Initio Modeling of Condensed Matter research line have expertise in first-principles atomistic, electronic and magnetic structure modelling of problems in bulk solids, surfaces and nanostructures and their recent research addressed four main areas: (i) semiconductor materials for photovoltaics and radiation detection, (ii) photocatalysis in biocompatible material, (iii) surface science of SiGe systems, and (iv) group-IV semiconductor alloys.

The Complex Networks systems research line determined the relaxation rate of the synchronization in the Kuramoto model in networks. The first report on the protein interaction network in human testis was provided. Hierarchical organization of finite components in directed networks such as Wold Wide Web, Twitter, brain networks was revealed. The theory of the k-core pruning process in complex networks was developed. It was shown that correlations between links lead to multiple hybrid and recurrent phase transitions in complex networks.

The Molecular Simulation research line made studies of phase transitions of magnetic ordering and of emergence of cooperative behaviour in social games in directed lattices and networks. Mean-field approximations to describe Monte Carlo simulation results have been proposed. Thermodynamic properties of C60 systems are also being studied.

The Quantum Transport research line addressed effects of geometric frustration on transport phenomena and magnetic behavior at the nanoscale. A new method of construction of exact localized many-body electronic eigenstates in decorated lattices was proposed. Anomalous superconductivity in low dimensional systems was also studied.

Overview of the research done by the NMBS group in the last two years

M.A. Valente1*, L.C. Costa1, F.M. Costa1, M.P.F. Graça1, F. Amaral2 , E.V. Ramana1, J. Suresh Kumar1, N.M. Ferreira1, K. Pavani1, F. Rey-García1

1Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal, 2Polytecnic Institute of Coimbra, 3000-271 Coimbra, Portugal

**mav@ua.pt*

The work done by the group "Novel Materials and Bio-Systems" in the last two year can be divided in three areas: Preparation of materials for electronic, optoelectronic and energy applications; Their characterization and; Projects with the industry.

We prepared materials by: Laser floating Zone; Laser treatment of surfaces; Microwave processing of oxides at high temperatures and "cork" at low temperatures; Sol-gel; Auto-combustion; Spin-coating; High energy ball milling, sintering. Ebeam.

The main materials prepared and characterized by structural, electrical, magnetic and optical studies in the group were: Magnetic nanoparticles; Ferrites with possibility to have interesting dielectric properties, such as high dielectric constant, Ferrites for microwave absorption; Glasses and glass-ceramics with dielectric, magnetic, and/or optical properties; Glasses with optical and luminescence properties; Phosphors for photoluminescence; **Ferroelectrics and multiferroics** environment friendly (Lead-free) **in bulk and thin films for energy harvesting applications**: single phase, composite bilayers, flexible polymer based nanocomposites are investigated; Ferroelectric oxides for photocatalytic (PC) and photovoltaic applications; Thermoelectric oxides, in order to develop materials suitable for high-efficiency power generation under large temperature gradients; Oxyorthosilicates as laser host materials, Materials with high/colossal dielectric constant (and low loss) for energy storage; Study of the interaction of the microwaves in porcelain and stoneware; Polymer composites with carbon nanotubes and nanoparticles; Bioceramics of the calcium phosphate-based compounds (Hydroxyapatite) for bio applications.
The group led or participated in several projects promoted by industry as: Laser treatment of surfaces of different materials envisaging laser cleaning, engraving and repair; development of oven (gas and microwave) prototype for porcelain preparation (at high temperatures); microwave oven for "cure Cork" (at low temperature); Development of new coatings with antibacterial properties based on bioglass for applications in dental implants; The electrical polarization features, especially the charge storage ability, of calcium phosphate-based commercial powders (Hydroxyapatite).

I3N Aveiro: The main research activities of OO group

João Lemos Pinto

Department of Physics and I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal

The main research activities of the Optics and Optoelectronics group have been focused on novel fiber sensors for challenging environments, optical solitons studies, light propagation in micro-structured optical fibers and fiber-optic communication systems.
Micro-sensors for real time cell control and performance and management of large scale-batteries Lithium batteries have been developed within European consortium Sirbatt- Stable interfaces for rechargeable batteries [1].
Optical fiber sensors have been designed and implemented for biomedical applications, namely as non-invasive technology to central arterial pressure assessment and physical rehabilitation, in collaboration with Instituto de Telecomunicações- Aveiro, Centro Hospitalar Baixo Vouga and Centro Hospitalar e Universitário de Coimbra [2].
An optical platform for multi-parameter monitoring of Madeira wine has been further developed in collaboration with FCEE, UMa, for physicochemical characterization and industrial vinification and ageing process studies [3].
Some theoretical studies have been carried out on the existence and stability of optical solitons and the light propagation in micro-structured optical fibers, towards generation of UV light or supercontinuum light [4].
Finnaly, space-division multiplexing has been proposed to increase capacity in fiber-optic communication systems by allowing transmitting several parallel data streams through a single fiber, using orthogonal modes of a few-mode fiber or multiple cores in a multicore fiber [5].

References

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POSTER PRESENTATIONS

3D printing of materials and its applications

Inês Ropio[1], Ana Gaspar[1], António Almeida[1], Paulo Duarte[1], Catarina Bianchi[1], Filipe Silvestre[2], Ana Baptista[1] and Isabel Ferreira[1]

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This work reports the possibilities of 3D printing techniques to perform advanced materials with customized designs. Polymeric and aqueous base pastes have been used to obtain 3D objects by extrusion or stereolithography (SLA). Important progress has been made towards obtention of very hard 3YSZ ceramic pieces using powders supplied by INNOVNANO. Flexible polymeric aesthetic prothesis implants in collaboration with Estefania Hospital were made and new biocompatible resins for SLA printers produced. This activity made possible a collaboration with Champalimaud Foundation and a P2020 project.

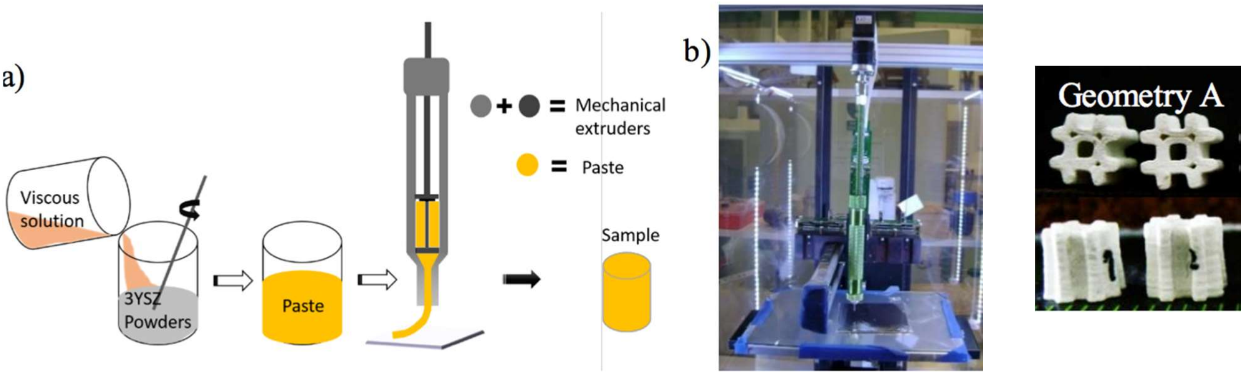

Fig. 1. Extrusion printer and ceramic pieces printed with UNINOVNANO 3YSZ powders [1].

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1-ERC-2014CoG-647596, CapTherPV
2-HA2020, RIA, 2014, 645241, TransFlexTeg

Atomistic and heat dissipation modelling of carbon nanostructures

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Molecular dynamic simulations have been employed to study bonding in carbon nanostructures. We calculate the forces between particles with the atomistic C-C potentials (for ex: Adaptive Intermolecular Reactive Empirical Bond Order potential (AIREBO), with nondivergent Morse potential[1]), and we consider a Langevin thermostat. We calculate the Potential of Mean Force (PMF(r)) between the two centers of mass (CoM). We are particularly interested in the behavior of PMF(r) at short distances and on its dependence on temperature. The interaction of rotational and vibrational degrees of freedom with the CoM distance may lead to a temperature dependence of PMF(r). Molecular simulations of fullerite were previously done using two body, temperature independent interaction potentials with which we can compare.

A structure of diamond nanoplatelets, coated with a graphite layer, vertically aligned over a nanocrystalline diamond film, was grown on a silicon substrate[2]. In this work, finite element simulations were used to study the heat dissipation properties of such a structure. Natural and forced convection conditions were considered. The small dimensions of the systems introduce an extra complexity, in particular, the mean free path of the air molecules becomes comparable with the distances between neighboring platelets. Depending on the Knundsen numbers, the continuum assumptions behind the traditional fluid dynamics equations may have to be discarded. In an intermediate case, the Navier-Stokes equations can be used along with appropriate boundary conditions.

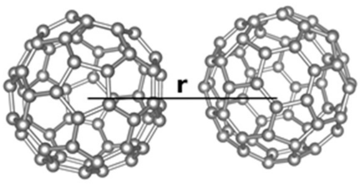

Fig. 1.A) Dimer formed by two C60 molecules with the CoM at a distance **r**.

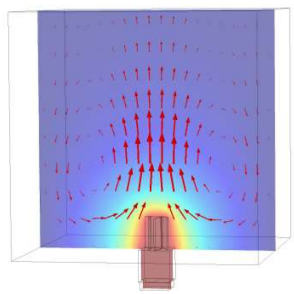

Fig. 1.B) Heat dissipation by convection. The system is in a stationary state.

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Bioinspired heterogeneous elastic microfilaments

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Helical-shaped filaments are ubiquitous in nature at various scales ranging from tendrils with millimetric diameters to proteins. The understanding of the mechanisms that lead to elastic nature and manmade filaments, like plant stems and polymer networks, to adopt a helical configuration is crucial to produce structures with specific helical geometries[1]. In the case of plant tendrils, neither the helical pitch nor the radius are constant, indicating the variation of the intrinsic curvature along the stem. Another typical occurrence happens when tendrils attach to a support and start to curl. Since both ends are fixed and cannot rotate, perversions inverting the handedness arise to balance the overall twist. In this work, we studied how the geometry of electrospun filaments can be precisely shaped. This striking and innovative behavior is observed when one side of stretched filaments is irradiated with UV light, modifying their outer-surface mechanical properties. Upon release, the regions with higher curvature start to curl first, while regions with lower intrinsic curvature remain stretched until start to curl later. The results presented here are important to understand why structures adopt a helical shape in general, which is of interest in nanotechnology, biomolecular science, or even to understand why plant filaments curl.

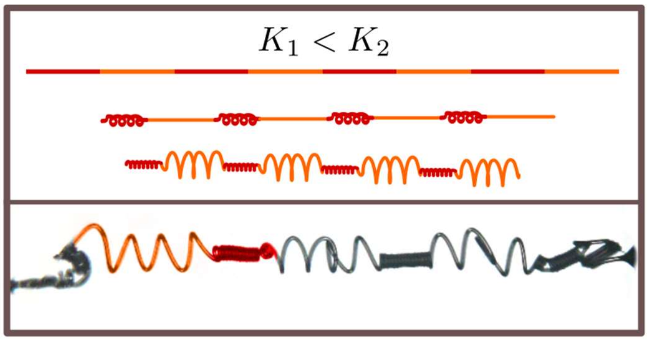

Fig. 1. Electrospun fibres with multiple intrinsic curvatures.

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Biosensor research activity at CENIMAT/i3N

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Biosensors are defined as analytical devices incorporating a biological material intimately associated with or integrated within a physicochemical transducer or transducing microsystem, which may be optical, electrochemical, thermometric, piezoelectric, impedimetric, magnetic or micromechanical. These devices have been applied to a wide variety of analytical problems in several scietific fields, such as medicine, biomedical research, drug discovery and point-of-care.

Here, we present different approaches for biosensor production and applications, currently under development at CENIMAT/I3N: (i) paper-based colorimetric sensors [1-3] for glucose monitoring, diagnosis of infectious diseases and bacteria detection; (ii) ion sensitive field-effect transistors [4] for direct gene expression-profiling platform; (iii) PDMS-based microfluidics for mixing of different solutions at small volumes [5] and optical detection of DNA sequences via gold nanoprobes [6] (iv) digital microfluidics based on the electrowetting-on-dielectric phenomenon for nucleic acid amplification in extremely small volumes (inferior to 2μL).

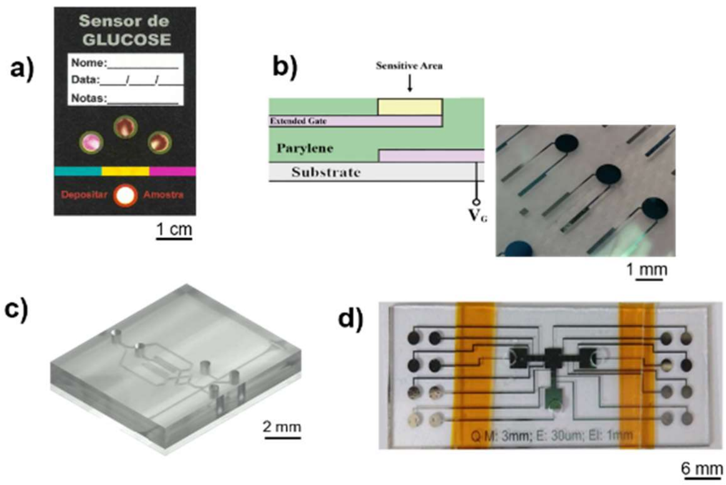

Fig. 1. Different approaches for biosensor production and applications, currently under development at CENIMAT/I3N: a) glucose paper-based sensor; b) ion sensitive field-effect transistor; c) PDMS-based microfluidics platform; d) digital microfluidics platform.

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Characterization and optical monitoring of Madeira wine production and ageing processes

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Madeira fortified wines are characterized by a peculiar production and ageing processes that can include heating (usually at 45 °C for 4 months) followed by ageing in oak casks placed in sunshine heated lodges. The high oxidative operating conditions contribute to the specific organoleptic characteristics and exceptional longevity, as 100 years old wines can easily be found and tasted. Made from 5 main grape varieties, fermentation is carried out following the empiric tradition of the producer, and stopped by the addition of grape spirit according to the desired sweetness and marketing characteristics. There is several challenging research issues that can be summarised as:

- The bouquet of these wines involves essentially tertiary aromas, namely spices, honey, dried fruits and jelly, where heating plays an important role in their formation. Although some terpenes can be detected, main aromas are more complex structures, such as sotolon. The thermal degradation reaction of sugars, mainly fructose, is involved in aroma formation, and thirty one related compounds were already identified [1]. Thus, the close monitoring of heating is an important issue.
- Ageing process is vital in order to assure that exceptional wines evolve for decades therefore modelling the ageing process is of utmost importance. The amount of data availabe regarding wines charcaterization makes the use of multivariate data analysis techniques advantageous to model ageing process and follow the wine evolution. Recently, it was proposed a new strategy to monitor the wine ageing process, namely the *Estufagem* process, based on wine chemical composition [2] .
- Intelligent monitoring of the vinification and ageing processes by new optical sensors for in loco measurements and decisions are therefore important.
- Global monitoring of the vineyards in order to detect undue chemical treatments and water stress, but specially the appearance of grapes rotting and other quality impacting diseases, appears as the following research objective.

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Chitosan-based Bio-nanomaterials @ CENIMAT/i3N

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Chitosan (CS) is the deacetylated form of chitin, a polysaccharide structurally similar to cellulose with vast biological and chemical attributes. In the Biomaterials' section of SBMG group from CENIMAT/i3N, chitosan is the base polysaccharide for the development of materials focused in two major biomedical applications: theranostic and tissue engineering.

Theranostic is defined as the combination of diagnostic and therapy agents in the same system. In the last years we have developed chitosan-based magnetic systems composed of iron oxide nanoparticles (Fe_3O_4-NPs) towards the production of multifunctional composite systems. In this work composite nanoparticles with magnetic core and chitosan shell are produced as drug delivery systems for doxorubicin (DOX) and magnetic hyperthermia agents for cancer treatment. [1-3]

Bone is a highly organized and specialized connective tissue with natural ability to self-heal and regain functionality. This capacity is, however, exposed to a great number of threats that can critically damage bone's health and trigger the need for bone substitutes. This work reports the production of new bone scaffolds for tissue regeneration using the Inverted Colloidal Crystal (ICC) geometry.Organic (chitosan/chitin nanowhiskers) and inorganic (hydroxyapatite) building materials were used to develop ICC scaffolds comprising ceramic, polymeric and composite matrices. [4-6]

In bone regeneration electrically charged surfaces enhances the osteointegration. Porous 3D scaffolds of CS and CS/hydroxyapatite (HA) were developed. Same samples were electrically polarized by DC contact. A comparative evaluation of non-charged, positively and negatively charged surfaces effect on bioactivity and in vitro tests with osteoblast was made. Negative surfaces show the best results.

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Crystallization in the ZnO –B_2O_3-SiO_2 glass system

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Glasses from the ZnO-B_2O_3-SiO_2 system have been widely studied and proved to be of great interest for the photonics area, since these materials are known to possess interesting photoluminescence properties, especially when doped with rare-earth ions or transition metals [1, 2]. It has also been reported that the crystallization of phases like zinc oxide (ZnO) or willemite, zinc orthosilicate (Zn_2SiO_4), within the glass matrix can be of great use to enhance photoluminescence properties and to serve as hosts for dopant ions, as long as the glass matrix maintains a high transparency.

The influence of ZnO/B_2O_3 ratio and thermal history on the crystallization behaviour of ternary ZnO-B_2O_3-SiO_2 glasses was studied by DTA, XRD, SEM and UV-Vis spectroscopy. Under specific heat-treatment conditions, transparent nanocomposite glass-ceramics were obtained.

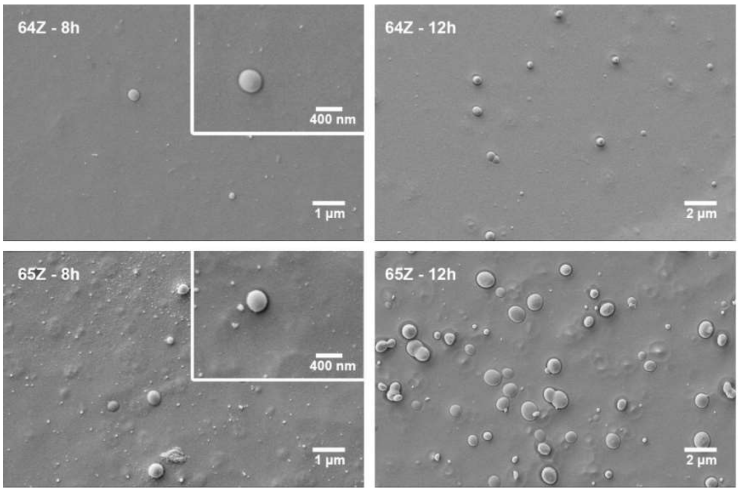

Fig. 1. SEM micrographs of the glasses heat-treated at 615 °C for different holding times.

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Cu(In,Ga)Se2 based Solar Cells: Dependence on the Cu Content

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The amount of Cu on Cu(In,Ga)Se_2 (CIGS) has a profound influence on the opto-electronic and on the structural properties of these layers. Such effect is also reflected in the electrical performance of resulting thin film solar cells. Most of the fundamental studies found in the literature are performed either in specimens based in crystals or in conventional co-evaporated thin films [1]. In the former case, the specimens lack the polycrystalline nature of the thin films that are used in solar cells. In the case of thin films produced by co-evaporation processes, like the three-stage growth process or other in-line processes, they usually present thin films that have a [Ga]/([Ga]+[In]) (CGI) depth profile and/or Cu-rich to Cu-poor transitions during the different growth stages. In this work, we prepared a set of CIGS samples using flat evaporation rates which produced films with a constant value of [Ga]/([Ga]+[In]) (GGI) in depth and without any Cu-transitions. The samples were studied using several techniques: X-ray diffraction (XRD), scanning electron microscopy/energy dispersive spectroscopy (SEM/EDS), photoluminescence (PL), and Raman spectroscopy. The CGI contents studied were 0.53 (10.5 % efficiency), 0.71 (13.8% efficiency), 0.85 (15.1% efficiency) and 0.98 (14.5% effciency) with a fixed GGI of 0.3. For lower Cu contents, the electrical performance lowers together with a lowering of the crystal quality and an increase of the effect of fluctuating potentials, as observed by PL [2-5]. EQE measurements show that between CGI values of 0.53 and 0.85, the bandgap energy values increase with increasing Cu content. A relation between the electrical performance and the morphological and opto-electronic properties for multi-crystalline samples with depth-flat Ga ratios and no Cu transitions is demonstrated.

The authors acnowledge P. Szaniawski, V. Fjällström and M. Edoff from the Uppsala University for supplying the CIGS samples and discussion of the results.

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Cultural Heritage Studies developed at CENIMAT/I3N Metals, Ceramics, Mortars and Stones

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Cultural Heritage studies involve the study of materials and manufacturing techniques of artefacts and built heritage, as well as the development of strategies and new materials for their conservation and restoration. For that purpose advanced characterization techniques are employed to study the chemical composition, phase constitution and structural information, which allows to understand degradation phenomena and ageing mechanisms.

In the case of metal artefacts, two of the most recent studies will be presented. The first compromise the materiality of Historical bronze bells, namely the composition and properties of high tin bronzes, as in the specific study of the Coruche bell, the oldest bell found in the Portuguese territory [1]. The second study is about the composition and microstructure of silver coins from the 16th century, which has allowed for the first time to infer about superficial microheterogenities of manufacturing origin which affects the surface elemental composition of high silver alloys [2].

In ceramic materials the case study to be presented refers to the unique majolica-type polychrome high relief tiles from 19th century from the UNESCO World Heritage Pena National Palace (Sintra, Portugal) [3-4].

In the case of mortars and stones three examples will be presented. Binders, mortars and conduit crusts from the Roman Aqueduct of Carthage in Tunisia from the 2nd century [5]; original and reconstruction period materials from the fortress of Safim in Morrocco (16th century); and reconstruction materials from the UNESCO World Heritage Minoan Knossos Palace in Creete (Greece) under the European Union Horizon 2020 HERACLES project [6].

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Development of fiber sensors network for measuring characteristic parameters in Li-ion cells

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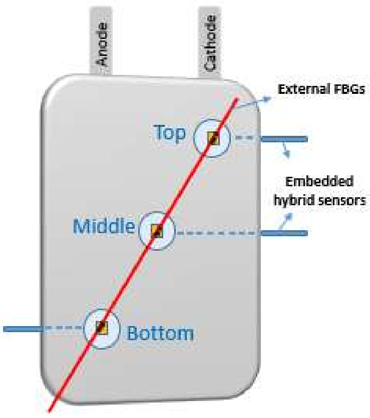
Lithium batteries have been extensively studied and used in many different applications, including power sources for renewable energy facilities and nuclear power plants where there are very high requirements in terms of security and reliability [1, 2].

Different sensing networks based on fiber Bragg gratings (FBGs) and Fabry-Perot (FP) cavities have been developed and tested for internal and external real-time monitoring of characteristic parameters in Li-ion pouch cells, such as temperature and strain. Temperature and strain sensitivities of 9.01 pm/ºC and 1.26 pm/με for the FBG sensor and 0.05 pm/ºC and 6.07 pm/με for the FP sensor were respectively obtained (see Fig.1).

The operation under various charge and discharge conditions such as high current, short circuit and over-charge has been studied. The fiber sensors were placed in specific positions of the pouch cells, in order to achieve an optimized design. Using the matrix method it was possible to discriminate internal strain and temperature. A comparison between external and internal temperature variations was also performed.



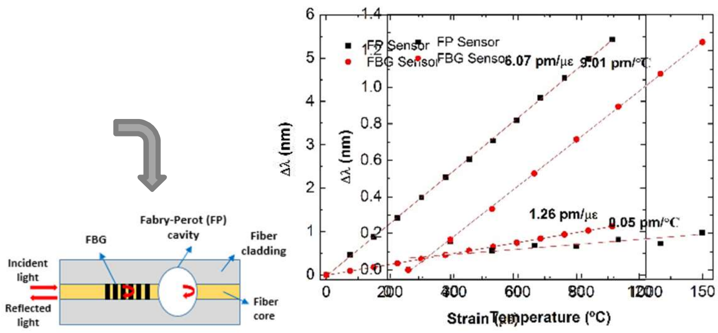


Fig. 1. Schematic diagram of the network sensors location in the Li-ion pouch cell and the hybrid sensors temperature and strain calibrations.

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Electrical properties of lithium ferrite particles embbebed in PLA matrix

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The goal of this work is to evaluate the electrical properties of the lithium ferrite, $LiFe_5O_8$, (LFO) particles powders embedded in a poly(lactid acid) matrix, with different weight concentrations, 3.5, 5, 8.5, 9.5, 19.5% (wt/wt). $LiFe_5O_8$, has interesting electrical and magnetic properties that's why is so used in technological applications. In this work, LFO powders were synthetized using lithium and iron nitrates as raw materials by solid state method and then heat treated at 1100 ºC [1].

AC measurements were performed using a Alpha-N broadband impedance analyzer (Novocontrol GmBH), in a range of frequencies from 10^{-1} up to 10^6 Hz. The temperature was increased from -35 ºC up to 140 ºC, in steps of 5 ºC. The DC measurements were extrapolated using the AC results, at low frequencies (f=0.1 Hz). In the samples with low LFO concentration, the impedance spectroscopy results are characterized by the detection of two relaxations: a dominant α process, associated with the dynamic glass transition, and a secondary process. Both are influenced by conductivity. The α relaxation process becomes broader as the concentration of LFO particles increases. For the samples with high LFO content the dielectric properties are dominated by the conductivity. The temperature dependence of the detected relaxation processes and conductivity was analysed, allowing the construction of a relaxation map, which provides the dynamic fingerprint of the material.

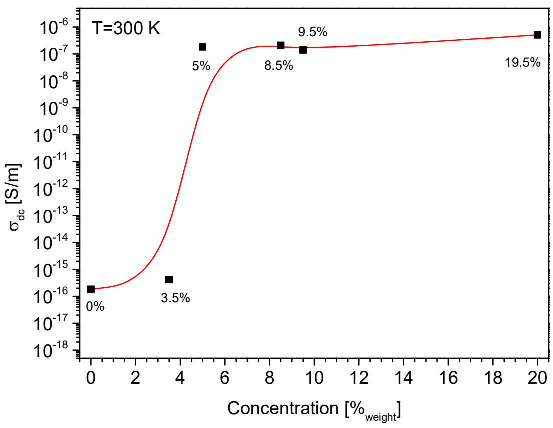

Fig. 1. DC electrical conductivity (σ_{DC}) at T=300 K, as a function of the LFO particles concentration.

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Electrospun fiber mats from polycaprolactone, chitosan and gelatin based materials as scaffolds for tissue engineering

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Combining polymers either through blending or synthesis of new functionalities yields materials with superior physical, chemical and biological properties. In this work, a polyester (polycaprolactone, PCL) was combined with two natural polymers (chitosan, CS, and gelatin, GEL) following two different route. In the first route, CS/PCL and GEL/PCL were blended using acetic acid with a small percentage of water as solvent. These solutions were electrospun in order to produce fibrous scaffolds. Scaffolds containing GEL were crosslinked with vapour phase glutaraldehyde (GTA). In the second route, segmented poly(urethanes), PU-CS and PU-GEL, were synthetized using PCL-diol as soft segment and the natural polymers as well as different dimethylol propionic acid:CS ratios as chain extenders. All PUs were dissolved in a mix of N,N-dimethylformamide and tetrahydrofuran to produce electrospun scaffolds.

The scaffolds were characterized regarding their morphology, water contact angle, mechanical properties, chemical bonds and were further tested *in vitro* for cell adhesion, growth and morphology of human foetal fibroblasts. All scaffolds display the typical morphology of non-woven fibre mats.

Results for the polymer blending scaffolds show: a hydrophilic behavior, the occurrence of cross-linking reactions of GTA with GEL in GEL/PCL and a higher elastic modulus (48 MPa) for CS/PCL. Cell adhesion in PCL/GEL was double that observed in PCL/CS. Cells proliferated until confluence was reached in both scaffolds.

Urethane and urea linkages are present in both PUs and their scaffolds have a hydrophobic character. The Young's modulus increased with the CS content in the PU-CS scaffolds but it is higher for PU-GEL (5.2 MPa). Only the scaffolds made from PUs containing natural polymers supported cell adhesion and proliferation.

Enhanced Polymer Light Emitting Diodes by energy transfer process in a simple device structure

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Polymer Light Emitting Diodes (PLEDs) have been attracting much attentions due to their low cost, easy fabrication process using the wet process, like Roll-to-Roll for large area emission and the possibility to obtain a simple and very bright emitter in all visible color spectra, towards lighting and signaling. In this work, PLEDs made by spin coating were extensively studied. PEDOT:PSS (Poly-(3,4-ethyleneioxythiophene):poly(styrene-sulfonate)) was used as hole injection layer and PFN (Poly [(9,9-bis(3'-(N,N-dimethylamino)propyl)-2,7-fluorene)-alt-2,7-(9,9–dioctylfluorene)]) as electron transport layer. The active layer was a blend of MDMO-PPV (Poly-(3,4-ethyleneioxythiophene):poly(styrene-sulfonate)) and Alq3, where the Alq3 wt.% changing from 5 to 20 %. MDMO-PPV exhibits a relatively strong emission in the orange spectrum region. In this work, we improve such emission by means of a transfer energy from the small molecule to the excited levels of MDMO-PPV as its absorption band can be easily overlapped by the Alq3 emission band. As no emission of Alq3 is observed we can assure that the carrier confinement inside the emissive layer is perfect. These results showed that the energy transfer from Alq3 to the MDMO-PPV is efficient and can be used as a basic principle for simple large-area emitters. The best result (and according to the current models for energy transfer from the bands overlapping) is obtained for 15% of Alq3. The bright increases upto five times (over 2000 cd/m^2 only at normal surface emission direction) and the efficiency increases up to twice, opening a new opportunity for large and efficient electroluminescent devices.

Fig. 1. Photograph of the PLED device

Enhancement of thermoplastic elastomer surface wettability

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The transfer and distribution of a fluid on a solid substrate depends, apart from other factors, on the surface tension (ST) of the fluid, and the surface energy (SE) of the substrate that will receive the fluid. For this reason, a surface treatment of the polymer substrate is normally needed due to its hydrophobic nature and low SE.

A novel surface treatment method in order to increase the SE is presented. Micro/nanosized silica particles (SP) are spread over the Thermoplastic PolyUrethane (TPU) substrate surface and thermally fixed. This step allows the SP sinking-in on the polymer surface, resulting in a higher polymer-particle interaction at their interfacial region. The addition of SP increased significantly the substrate SE and consequently the TPU wettability. Furthermore, SP shows a high affinity with the TPU due to the hydrogen-bond interactions between the silanol groups on the silica surface and the soft segments of the TPU [1]. Therefore, the developed treatment was effective on increasing the surface roughness of the substrate (by 621%) and increasing on the SE of the substrate (by 45 %). To the surface treated TPU substrate was applied conductive inks by inkjet printing (IP) and a significant improvement on the TPU printability was obtained (Fig.1).

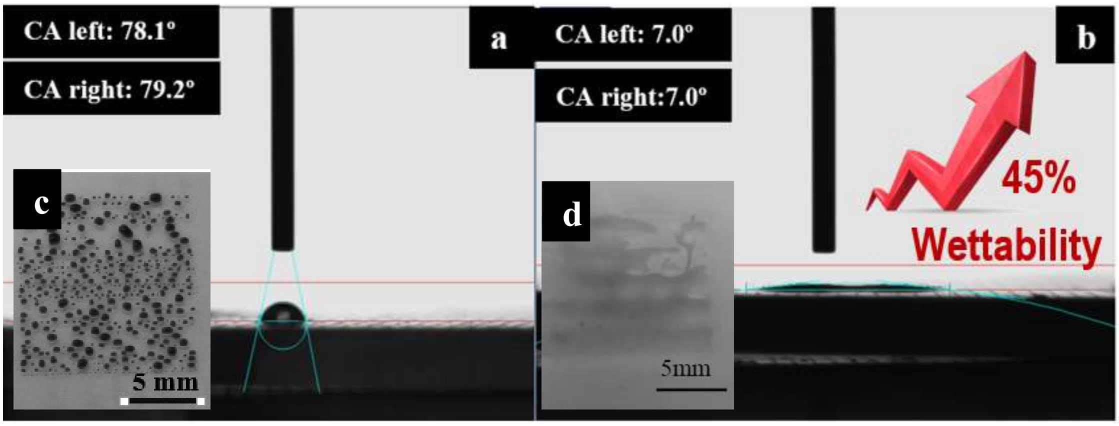

Fig. 1. Drop of water on the TPU substrate: a) before and b) after surface treatment. Conductive ink IP on the TPU susbtrate: c) before and d) after surface tretament.

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Exfoliation of grafite nanoplatelets for the preparation of nanocomposite films based on waterborne polyurethane, few layer graphene and carbon nanotubes

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Graphene and other carbon-based nanomaterials emerged as exciting materials revealing potential applications in various fields including in the polymer nanocomposites science. [1]

The production of graphene based on graphite exfoliation through non-covalent interactions with pyrene derivatives has been the focus of several studies, [2, 3] and was used for the exfoliation of graphite and stabilization in water of the produced few- and single- layer graphene without structural damage. The graphene suspensions may be mixed with water-soluble polymers and polymers that form stable suspensions in water such as waterborne polyurethane (WPU), a synthetic polymer used as high quality surface coating, providing an eco-friendly process without emission of volatile organic compounds (VOCs). [4]

The production of few-layer graphene (FLG) was performed through non covalent exfoliation of natural graphite in aqueous media using a pyrene derivative (PY). The evaluation of the extension of exfoliation was analyzed by Raman spectroscopy and X-Ray diffraction. After the exfoliation process of graphite with PY, bilayer and few-layer graphene were identified by Raman spectroscopy. X-Ray characterization reveals that the PY exfoliated graphene forms a powder that present a crystallographic structure that is different from both the structure observed for the PY only, obtained in similar conditions, and the as received graphite.

Few-layer graphene (FLG)/WPU, carbon nanotubes (CNT)/WPU and FLG/CNT/WPU nanocomposites were produced with incorporation of loadings of 0.025, 0.05, 0.1 and 0.5wt.%. The mechanical, electrical and barrier properties of the nanocomposite films were evaluated.

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Fabrication of lead-free ferroelectric oxides for energy harvesting applications

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Piezoelectric materials have widely been used to fabricate actuators, sensors and transducers. In these applications traditionally used materials are lead-based, which have stronger piezoelectric properties. However, in view of toxicity of lead during processing, there´s an increasing demand to replace lead based oxides with lead-free ones. This lead to rigorous studies on variety of Pb-free oxides with improved piezoelectric properties such as $(Na,Bi)TiO_3$-$BaTiO_3$, $(K,Na)NbO_3$, SiO_2, AlN, $LiNbO_3$, Aurivillius family of oxides. In these studies, it was found that lead-free solid solutions with the coexistence of two distinct crystallographic phases show the strong piezoelectric response due to the isotropic flattering of a free energy profile associated with the cubic–rhombohedral–tetragonal triple point or the tricritical point. As a result, large piezoelectric coefficient ≥ d_{33}~600 pC/N, g_{33}~29x10^{-3} V m/N, and g_{31}=-6.5x10^{-3} V m/N observed. In view of these salient features, we studied lead-free ferroelectric oxides, viz. perovskites, polymers and Aurivillius phases, for their multifunctional properties.

In this study we grew high-quality perovskite piezoelectric and Aurivillius phases using electrophoretic deposition and pulsed laser deposition on different substrates such as flexible metallic foils (Pt and metglas) and rigid substrates for their integration into electronics. We present details of fabrication, challenges in the growth of these films and results; structure, piezoelectric and multiferroic characterization of these materials for their use in energy harvesting applications (piezoelectric and photovoltaic).

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Fractional Viscoelastic Models

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In this work we discuss the connection between classical and fractional viscoelastic Maxwell models, presenting the basic theory supporting these constitutive equations, and, establishing some background on the admissibility of the fractional Maxwell model. We then develop a numerical method for the solution of two coupled fractional differential equations (one for the velocity and the other for the stress), that appear in the pure tangential annular flow of fractional viscoelastic fluids. The numerical method is based on finite differences, with the approximation of fractional derivatives of the velocity and stress, being inspired on the method proposed by Sun and Wu for the fractional diffusion-wave equation [1]. We prove the solvability, study the numerical convergence of the method, and also discuss the applicability of this method for predicting the fluid flow behavior in a real concentric cylinder rheometer. By imposing a step-strain, we observed the different rates of relaxation obtained with different values of α and β (the fractional order exponents that regulate the nature of the material). The supremacy of these models over the classical ones is shown in fig. 1, where the fit to the experimental relaxation modulus data of a polydimethylsiloxane sample is considered.

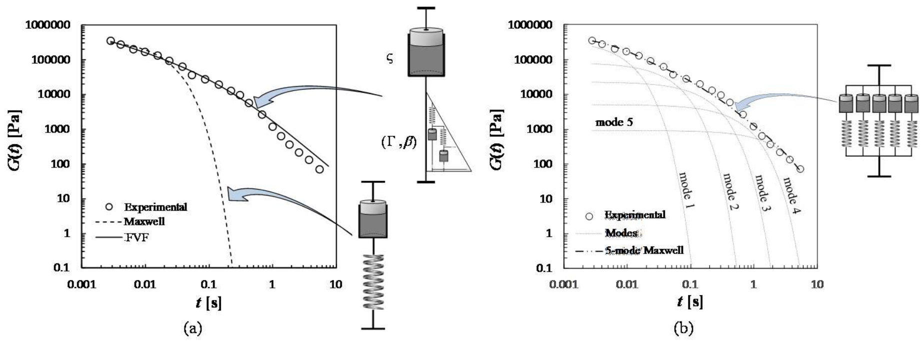

Fig. 1. (a) Fit of a single mode Maxwell model and the three parameter FVF to the experimental relaxation modulus data of a polydimethylsiloxane sample (the experimental data was adapted from [2]) (b) 5-mode Maxwell model.

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Gd and Lu oxyorthosilicates obtained by Laser Floating Zone for photonic applications

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Oxyorthosilicates have been employed as laser host materials during recent years due to their high chemical stability and the possibility to incorporate high concentrations of rare earth ions that allows modulating laser emission wavelengths. The aim of this work is the production of the gadolinium (GSO) and lutetium (LSO) oxyorthosilicates by the crucible-free Laser Floating Zone (LFZ) technique [1]. This method promotes a higher control synthesis in respect to conventional solid state methods like Czochralski (CZ) together with an important reduction on timing and fabrication costs.

GSO single crystal monoclinic fibres were obtained (Figure 1) as confirmed by a complete XRD analysis. On the other hand, quasi-eutectic ceramic samples formed by C2/c monoclinic LSO and $Ia\bar{3}$ cubic Lu_2O_3 phases were obtained from Lu derived orthosilicates, as was identified by Raman and XRD analysis. The optical characterization, accomplished by photoluminescence and photoluminescence excitation and accompanied with optical transmission studies suggests that the produced fibres are promising candidates to be doped in order to develop new highly efficient laser materials or to be applied as UV light sensors.

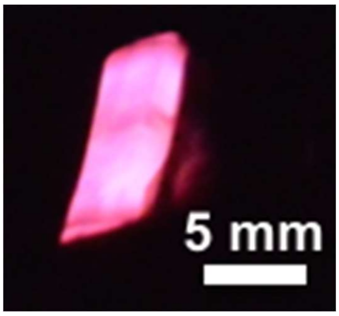

Fig. 1 a) Image of the red emission of the GSO crystal under 275 nm excitation, b) SEM micrograph of the quasi-eutectic LSO ceramic.

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Graphene synthesis and funcionalization: batteries and supercapacitors applications

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Green synthesis of graphene is a challenging research topic that has been addressed by the authors focusing its application in batteries and supercapacitors. Results of electrochemical and chemical exfoliation of graphite are shown. Planar supercapacitors were made by laser reduction of graphene oxide and its characterization performed by Cyclic Voltammetry. The graphene obtained by the different methods is compared using the Raman technique. The performances of cellulose based electrochemical devices are also presented.

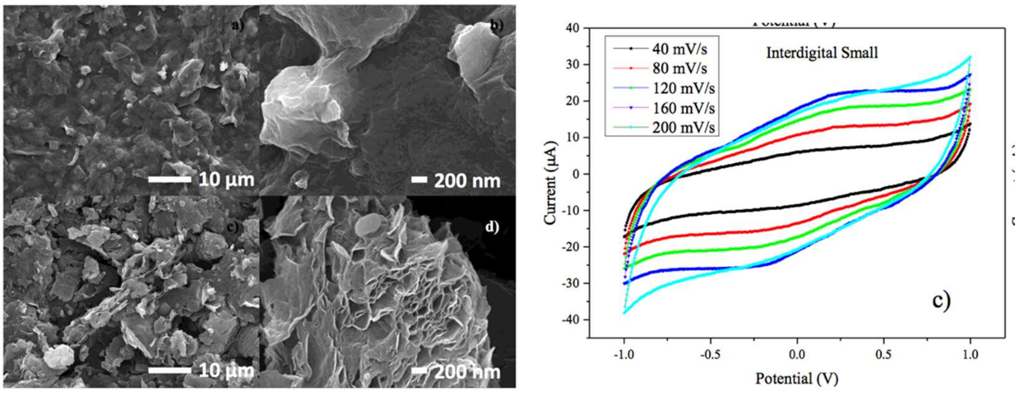

Fig. 1. Laser reduction of GO and its application for supercapacitors [1].

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2-HA2020, RIA, 2014, 645241, TransFlexTeg

Hybrid Polyamide Micro- and Nanoparticles for Multifaceted Applications

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This project explores a recently patented versatile method for the synthesis of loaded polymer micro- and nanoparticles [1] and suggests two possible lines for their application. The method is based on activated anionic ring-opening polymerization (AAROP) of lactams carried out in a solvent, in the presence of the finely dispersed payloads. Particles based on polyamide 4 (PA4), polyamide 6 (PA6), and polyamide 12 (PA12) were produced, carrying diamagnetic or paramagnetic metals, metal oxides, carbon allotropes or other organic or inorganic components not impeding the AAROP. The one-pot synthesis allows the simultaneous polymerization of various lactams forming copolymeric particulate systems with mixed payloads. The particles are mesoporous, with typical sizes of 0.5–50 μm, depending on the lactam and payload types, catalytic system and the reaction parameters. (Figure 1a)

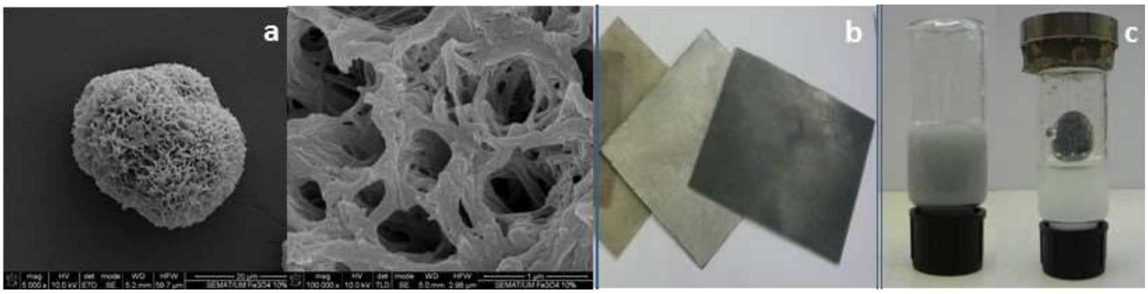

Fig. 1. (**a**) Typical particle sizes and porosity; (**b**) hybrid composite plates from loaded particles; (**c**) magnetic particles for biomedical applications

The results of this project show that fine-tuning of the propeties of the loaded particulate systems enables adjustement to specific industrial or biomedical applicatons. Thus, compression molding of metal/carbon loaded PA6 or PA12 particles produced polyamide hybrids combining magnetic susceptibility and electroconductivity (Fig. 1b). The biocompatible PA6 or biodegradable PA4 particles (Fig. 1c) are being tested for enzyme carriers, green catalysts and in stimuli-responsive smart drug delivery systems.

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Improving detector-grade SiC by defect engineering: a first-principles study

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Silicon carbide (SiC), one of the most promising wide-bandgap (2.0 eV $\lesssim E_g \lesssim$ 3.4 eV) semiconductors for making devices to be subject to harsh (high-temperature, highly corrosive, and high-radiation) environments [1]. It is also known that *grown-in* carbon vacancies have a huge impact in limiting the minority carrier life-time of SiC, and therefore they are highly detrimental to the performance of SiC as a base-material for radiation and light detection. Based on recent indications that SiC-growth based on a chlorinated chemistry strongly decreases the presence of carbon vacancies [2], we started to investigate by means of atomistic first-principles methods, what are the most stable complexes involving isolated Cl, F, H and O defects in 4H-SiC (the polytype of choice for making detector diodes), as well as their interactions with intrinsic defects like the carbon and silicon vacancies. We show that oxygen is a promising passivation agent of carbon vacancies, particularly in n-type material, where it either behaves as a double donor or as an inert interstitial impurity. We also found that interstitial oxygen impurities can be introduced in the SiC and be made to react with the vacancies at moderate annealing conditions.

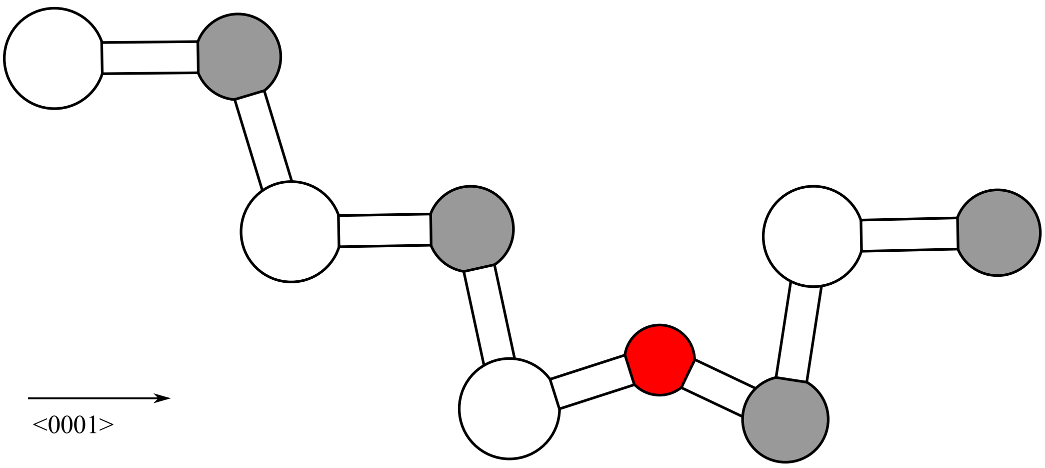

Fig. 1. Oxygen interstitial (O_i) structure in 4H-SiC. Oxygen, carbon and silicon are shown in red, grey and white, respectively.

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Increased Cell Proliferation and Metabolism by Electrical Stimulus on Nanocarbon Hybrid Platforms

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Nanocarbon allotropes are promising materials for electrically assisted tissue regeneration purposes due to their chemical inertness, biocompatibility, extreme mechanical properties, and, importantly, low and tailorable electrical resistivity. In this work, vertically aligned nanoplatelets of diamond (5 nm) coated with a graphite layer (100 nm) produced by the microwave plasma chemical vapor deposition (MPCVD) technique were explored as substrates for electrical stimulation of MC3T3-E1 preosteoblasts. The optimization of experimental synthesis parameters enabled the nanoplatelet vertical growth, an increased crystalline quality of the nanographite phase and a decrease of the electrical resistivity by over 1 order of magnitude.

The culture of the preosteoblasts on these templates was exposed to two consecutive daily cycles of 3 μA direct current stimulation. Improved cell proliferation and metabolism together with a high cell viability were observed after electric stimuli, Fig.1. Even in the absence of DC stimulation, this nanocarbon hybrid platform promotes an up-regulating effect of preosteoblastic maturation intrinsically exerted by the nanoplatelet sutucture, as indicated by the increased alkaline phosphatase (ALP) activity.

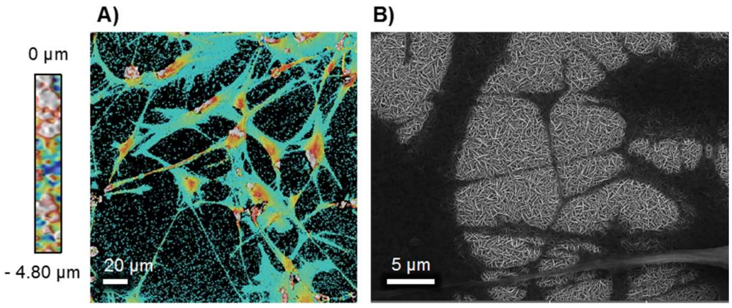

Fig. 1. a) Cell morphology and anchorage of electric stimulated MC3T3-E1 preosteoblasts grown on diamond nanoplatelet surfaces after 3 days of culture. A) Representative high Z-resolution optical profillometry image. B) Representative SEM image.

This work was performed under the colaboration of M. Cicuéndez, V. S. Silva and M. Vila, from Research unity of TEMA-NRG and Associate Laboratory of CESAM, University of Aveiro.

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In-line rheo-optical characterization of polymer systems at constant extrusion conditions

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As it is increasingly important to minimize costs and time-to-market when developing polymer systems with improved performance, in-process characterization methodologies become more attractive. Indeed, it is important to make available fast response characterization tools albeit using small amounts of sample are capable of generating relevant data on the rheological response, process-induced material structure and product properties. Recently, the authors developed a prototype modular small-scale single / twin-screw extrusion system with outputs in the range of grams/hour that was coupled to a rheo-optical slit die adequate to measure shear viscosity and normal-stress differences and perform optical measurements [1]. As with most similar attempts, the generation of a range of shear rates implied operating the extruder with varying screw speeds or feed rates. However, this changes the thermomechanical experience of the material inside the machine and, henceforth, may change the characteristics of the material the die inlet, which in turn may jeopardize the validity of the measurements. To circumvent this problem, the authors adopted a design concept that has been seldom utilized, consisting of a die with two perpendicular channels, each fitted with an output control valve at its inlet, the total pressure drop remaining constant. While one of the channels can be utilized for conventional extrusion, the other has a slit configuration and adequate for rheo-optical characterization (Fig. 1). This solution is validated and several case studies (polymer blends, polymer nanocomposites and biodegradable polymers) are discussed.

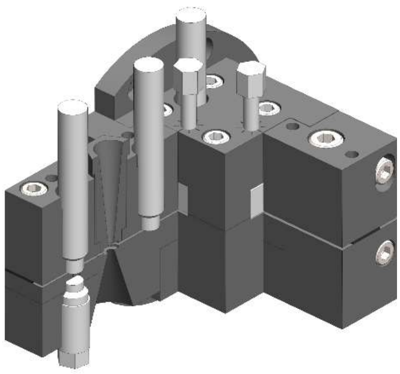

Fig. 1. New Rheo-optical slit die

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Innovation towards the fabrication of silicon solar cells on paper

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The growing interest in exploring thin film technologies to produce *n-i-p* silicon solar cells on low cost substrates (such as plastic, ceramic and more recently, paper), with outstanding performances and capability to address the energy market needs, turns the optimization of their fabrication process a key area of development. A combination of design of experiments, experimental data, computer simulations and statistical analysis, provides the tools to explore in a multidimensional fashion the interactions between fabrication parameters and maximize the expected experimental outputs. [1][2] Further improvements in the solar cells efficiency can arise from the application of optimized light trapping structures on the device rear and/or front contact, to boost their photocurrent generation via optical path length enhancement inside the silicon layer. [3]

Moreover, when dealing with exotic substrates, such as cellulose-based substrates, additional challenges arrise. Among the most critical challenges is the substrate roughness and porosity, which often hinders the quality of the electrical devices and short-circuits solar cells. Developing novel coating methods (to eliminate porosity and planarize the paper surface) and monitoring in real-time the fabrication process (to improve the device quality), are noteworthy strategies to approximate the solar cell efficiency to those fabricated on regular substrates. [4][5].

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Iron oxide based nanoparticles embedded in silica and polymeric matrixes

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Iron based magnetic nanoparticles have been widely investigated for their great potential for biomedical applications such as hyperthermia or delivering drugs and other applications like microwave absorber. For improving biocompatibility and reduced nonspecific magnetic binding it is a prerequisite to embed the nanoparticles with a "inert" layer. In this work innovative preparation methods, sol-gel based routes and laser floating zone were employed to prepare Fe_2O_3, Fe_3O_4 and $MnFeO_2O_4$ nano particles and further encapsulate them in a glassy silica and in a polymer matrix. Moreover, auto-combustion synthesis method was also used to prepare Fe_2O_3, Fe_3O_4 and $MnFe_2O_4$-silica nano composite. The morphological, structural, electrical, dielectrical and magnetic properties of the nano composites were investigated keeping in mind their future biomedical applications as hyperthermia agents and anticancer drug delivery with the ability to attain magnetic guidance to the therapeutic site.

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Kirigami of self-folding structures

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Self-assembly processes provide a natural approach to highly parallel fabrication of complex structures [1,2]. Three-dimensional shells can be synthesized from the spontaneous self-folding of two-dimensional templates of interconnected panels, called nets, as shown in Fig 1. The yield is maximized following sequentially two design rules: (i) maximum number of vertices with a single-edge cut and (ii) minimum radius of gyration of the net. Previous methods to identify the optimal net are based on random search and thus dependent on the number of sampled configurations and limited to very simple shell structures [1]. Here, we show that the optimal net can be found deterministically. We map the connectivity of the shell into a shell graph, where the nodes represent the vertices and the links the edges. By applying the design rule (i), we reduce the search to finding the set of maximum leaf spanning trees of the shell graph, to which (ii) can be applied straightforwardly. By reducing the search space this procedure allows to designing much larger shell structures, since the fraction of nets satisfying criterion (i) is very small, and decays exponentially with the shell graph size, see Fig 2. Furthermore, our method allows to apply additional design rules, such as shells containing holes, see Fig 1.

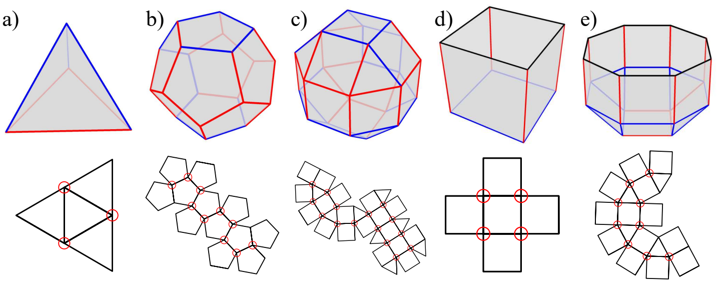

Fig. 1. Optimal nets for various example shells. Shells a), b), and c) are closed, while d) and e) have one hole.

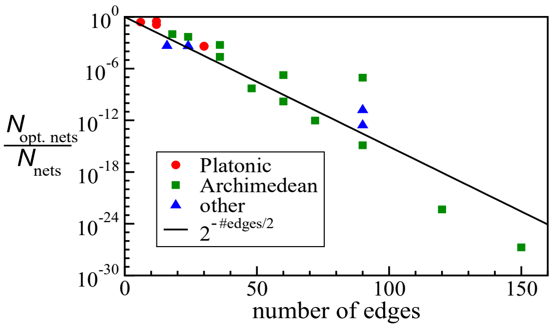

Fig. 2. Fraction of nets with maximum number of vertices with a single-edge cut.

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Laser ablation in liquids: an effective strategy in the synthesis of upconverting NPs for bio application

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Inorganic nanoparticles (NPs) doped with trivalent lanthanide ions (Ln^{3+}) showing the ability to undergo up-conversion (UC) mechanisms when pumped with near infrared (NIR) light, are suitable alternatives to replace the conventional materials used currently in biological labeling. The emission of visible light within the biological optical window, under NIR excitation, allows minimizing problems related to the low penetration depth of the excitation radiation, autofluorescence and damage of the tissues that occur under ultraviolet/visible excitation. Typically, chemical strategies are applied to produce the UC NPs, but these are frequently time consuming processes and give rise to NPs with low purity, unsuitable for biological applications. The pulsed laser ablation in liquids (PLAL) technique appeared recently as an alternative and effective strategy to produce UC NPs [1]. The possibility to produce pure and stable colloidal solutions in biocompatible solvents is one of the main advantages of PLAL. In this work, ZrO_2 NPs doped with different lanthanide ions, namely trivalent thulium (Tm^{3+}), erbium (Er^{3+}) and holmium (Ho^{3+}), were produced by PLAL in water. The as-produced spherical NPs show intense UC emission at room temperature, in the visible and NIR spectral range, characteristic of the intraionic transition of each dopant ion, when excited with 980 nm photons. The role of dopant concentration and co-doping with Yb^{3+} ions in the UC luminescence was investigated.

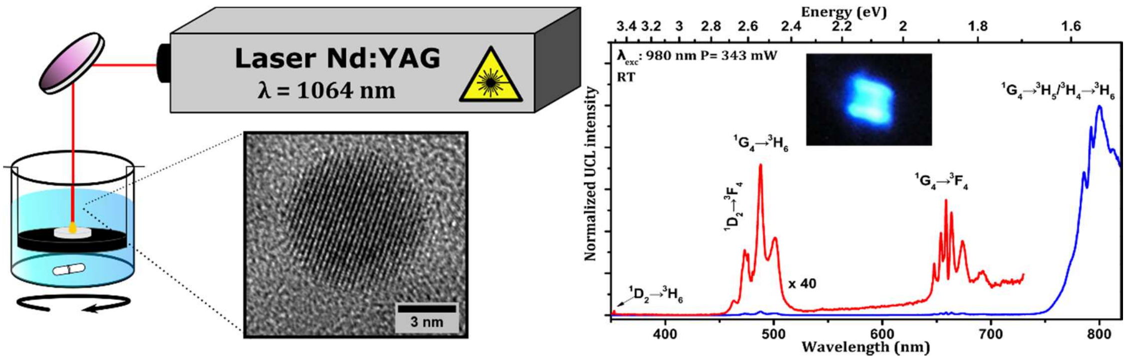

Fig. 1. Representation of the experimental setup used on PLAL. TEM imagem of Tm^{3+}, Yb^{3+} co-doped NPs and respective emission spectrum obtained upon 980 nm photon excitation [1].

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Light-induced non-thermal population of optical phonons in nanocrystals

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Raman spectroscopy is widely used to study bulk and nanomaterials, where information is frequently obtained from spectral line positions and intensities. In this study, we monitored the Raman spectrum of ensembles of semiconductor nanocrystals (NCs) as a function of optical excitation intensity (*optical excitation experiments*). We observe that in NCs the red-shift of the Raman peak position with increasing light power density is much steeper than that recorded for the corresponding bulk material. The increase in optical excitation intensity results also in an increasingly higher temperature of the NCs as obtained with Raman thermometry through the commonly used Stokes/anti-Stokes intensity ratio. More significantly, the obtained dependence of the Raman peak position on temperature in optical excitation experiments is markedly different from that observed when the same NCs are excited only thermally (*thermal excitation experiments*). This difference is not observed for the control bulk material. Thus, under moderate/strong optical pumping there is an additional contribution to the Raman peak position in NC systems, which is unseen in bulk materials. The inefficient diffusion of photogenerated charges in nanoparticulate systems, due to their inherently low electrical conductivity, results in a higher steady-state density of photoexcited charges and, consequently, also in a stronger excitation of optical phonons that cannot decay quickly enough into acoustic phonons. This results in a non-thermal population of optical phonons and thus the Raman spectrum deviates from that expected for the temperature of the system. Our study [1] has major consequences to the general application of Raman spectroscopy to nanomaterials.

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Liquid crystal suspended droplets revealing plants cellulose micro/nano filaments morphologies

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In plants long coiled left-handed helicoidal filaments can be isolated from plants petioles tracheary [1]. The morphology as well as the interactions of these helices with the environment is crucial for the plant survival [2]. This work represents an extension of the work that the team has been developing in which the surface morphology of Natural micro/filaments can be revealed by liquid crystals [3]. We focus on helical micro/nano filaments isolated from *Agapanthus africanus* and *Ornithogalum thyrsoides*. Their composition is determined and the outer surface morphology probed by scanning electron microscopy (SEM) and by polarizing optical microscopy (POM) observations of nematic liquid crystal droplets pierced on the Natural filaments. The structures identified were correlated to the plant filaments morphologies. Tensile tests were performed on the studied filaments and a surprisingly unusual behavior was observed. This work can uncover new perspectives in the understanding of the mechanism, which drives the formation of left helices in plants such as in petiole tracheary elements.

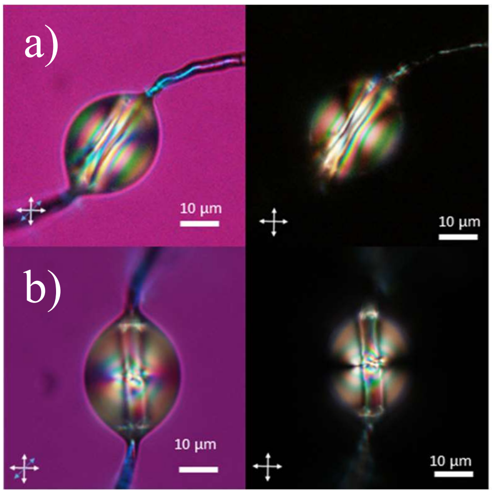

Fig. 1. Liquid crystal textures observed on suspended a) *A. africanus* and b) *O. thyrosoides* filaments.

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Magnetoelectric effect in composites based on single crystalline piezoelectrics

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This work presents a theoretical and experimental study of the anisotropic magnetoelectric (ME) properties of differently structured composites featuring piezoelectric (PE) single crystals, mainly lead-free, for diverse multifunctional applications. An averaging linear quasi-static model is shown to support the possibility of inducing large anisotropic ME voltage coefficients in composites comprising metglas and lead-free PE single crystals such as lithium niobate ($LiNbO_3$, LNO), lithium tantalate ($LiTaO_3$), gallium phosphate ($GaPO_4$, GPO), quartz (SiO_2), langatate ($La_3Ga_{5.5}Ta_{0.5}O_{14}$) and langasite ($La_3Ga_5SiO_{14}$) through the optimization of the crystal orientation. An experimental comparative study of the direct ME effect in simply bonded tri-layered laminates of metglas and LNO, GPO and PMN-PT crystals is exposed. Though PMN-PT has much larger charge piezocoefficients, the direct magnetoelectric voltage coefficient is found to be comparable in all of the composites due to a much lower dielectric permittivity of the lead-free crystals. Greatly enhanced ME coefficients in certain resonance modes are explored, and their relation to the material properties of the crystals and the geometry of the composites is investigated. We demonstrate that the control of the PE crystal's orientation can in principle be used to obtain almost any desired quasi-static and resonant anisotropic ME properties for any given application.

Bi-layered composites comprising PE bidomain plates of 127ºY-cut LNO were further studied for applications in low-frequency magnetic sensors. The LNO plates possessed an engineered bidomain structure with opposite spontaneous polarization vectors along the thickness direction. Impedance, ME effect and equivalent magnetic noise density measurements were performed on the composites operating under quasi-static and resonant conditions. ME coefficients of up to 578 V/(cm·Oe) were obtained at ca. 30 kHz at the bending resonance. Equivalent magnetic noise density measurements yielded values down to 153 pT/Hz$^{1/2}$ at 1 kHz and 524 fT/Hz$^{1/2}$ under resonant conditions. A further optimization of the fabrication techniques, laminate geometry and detection circuit is expected to permit reducing these values down to at least 10 pT/Hz$^{1/2}$ and 250 fT/Hz$^{1/2}$, respectively, and the resonance frequency by at least two orders of magnitude. Such systems may in future be very useful in simple and sensitive, passive and stable, low-frequency and high-temperature vector magnetic field sensors.

Mapping the Structure of Directed Networks: Beyond the "Bow-tie" Diagram

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We reveal a hierarchical, multilayer organization of finite components - tendrils and tubes - around the giant connected components in directed networks (Fig. 1) and propose efficient algorithms allowing to uncover the entire organization of key real-world directed networks, such as the World Wide Web, the neural network of Caenorhabditis elegans, and others. With increasing damage, the sizes of the giant components decrease while the number and size of tendril layers increase, enhancing the susceptibility of the networks to damage.

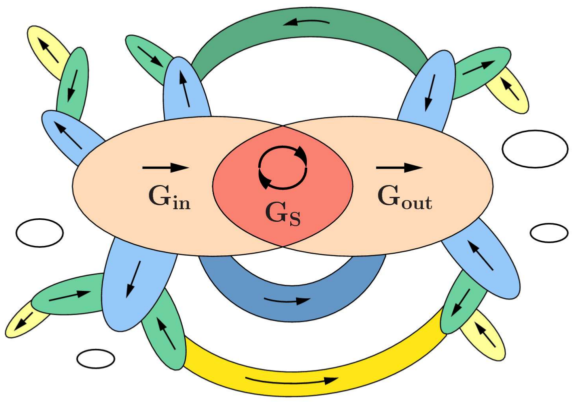

Fig. 1. Schematic view of the complete structure of a directed network with a giant strongly connected component (G_S), giant in- and out-components (G_{in} and G_{out}), and finite directed components (tendrils and tubes). Disconnected finite clusters are shown as open ovals. Different tendril layers are shown by different colors.

Medical systems based on scintillation materials

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Medical imaging and Radiotherapy are two important fields of Medicine that use ionizing radiation. Currently we are working in applications that cover both of these fields by using scintillation materials and solid state photomultipliers. One application is the development of a new concept of a preclinical Positron Emission Tomography (PET) scanner to be used for small animal imaging, to study human diseases and validate new drugs and therapeutics in animal models. This system uses, for the detection of the e^-e^+ annihilation position, cells composed by inorganic scintillators (LYSO) and Si photomultipliers, presenting state of the art position resolution over the whole field of view. The other application is the development of a radiation dosimeter to be used in prostate and breast brachytherapy, capable of providing real-time and in-vivo dose measurement, and presenting high sensitivity and no dependencies on energy, dose, dose rate and temperature, unique capabilities that cannot be found in any other dosimeter. This device uses, as the sensitive medium, a small (~1Øx3 mm) scintillation optical fiber coupled to a standard light-guide optical fiber and a SiPM for light readout. Present status of development of both systems and results of first clinical tests will be presented.

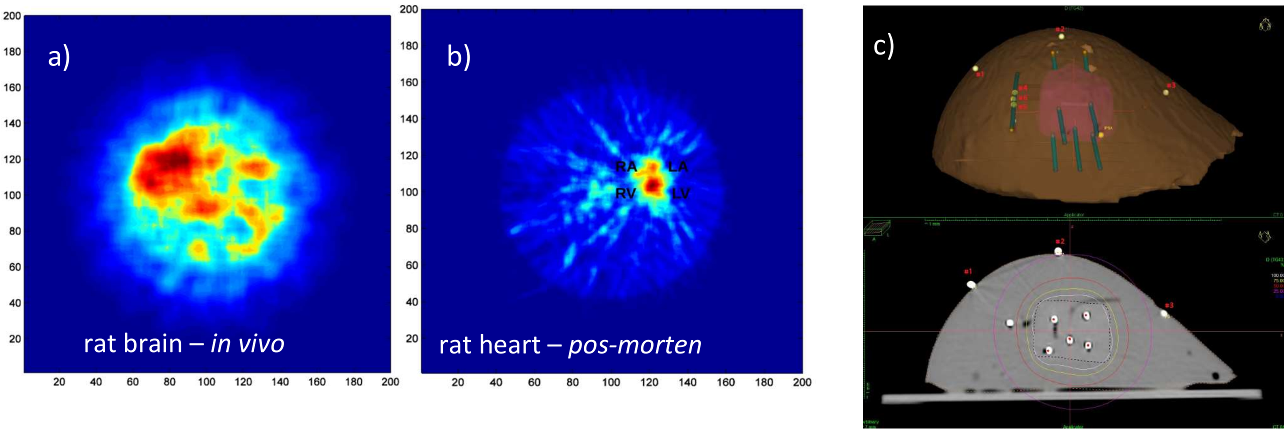

Fig. 1. a) and b) Examples of images obtained with the preclinical PET scanner. c) detail of the Oncentra Brachy 4.5.2 treatment planning software showing the breast phantom highlighting the 5 catheters, the one for the dosimeter probe with 3 reference positions plus 3 surface reference positions.

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Metal-oxide nanostructures synthesized under microwave irradiation

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The aim of environmentally friendly materials for multifunctional purposes and produced with low-cost production routes is a reality nowadays. Chemical synthesis routes are known to be inexpensive and versatile, where the hydrothermal/solvothermal synthesis using conventional heating or more recently under microwave irradiation are interesting options for the production of high quality nanomaterials. Comparing conventional heating to microwave synthesis, the former is usually inefficient, time and energy consuming, while the latter is relatively cheap due to its unique features such as short reaction time, enhanced reaction selectivity, energy saving, homogeneous volumetric heating and high reaction rate. In the present work, vanadium (VO_2), tungsten (WO_3), zinc (ZnO), zinc-tin (ZTO), copper (Cu_2O and CuO) and titanium (TiO_2) oxides were synthesized under microwave irradiation varying the synthesis parameters such as time, temperature, pressure, power input and solvent used. Several nanostructures such as spheres, stars, plates, whiskers, nanorods and nanowires were successfully synthesized (Figure 1) [1-3], where these nanostructures were further structurally characterized by scanning electron microscopy (SEM) and employed in optoelectronic devices such as thin-film transistors, electrochromic and thermochromic devices, sensors, and as efficient photocatalysts.

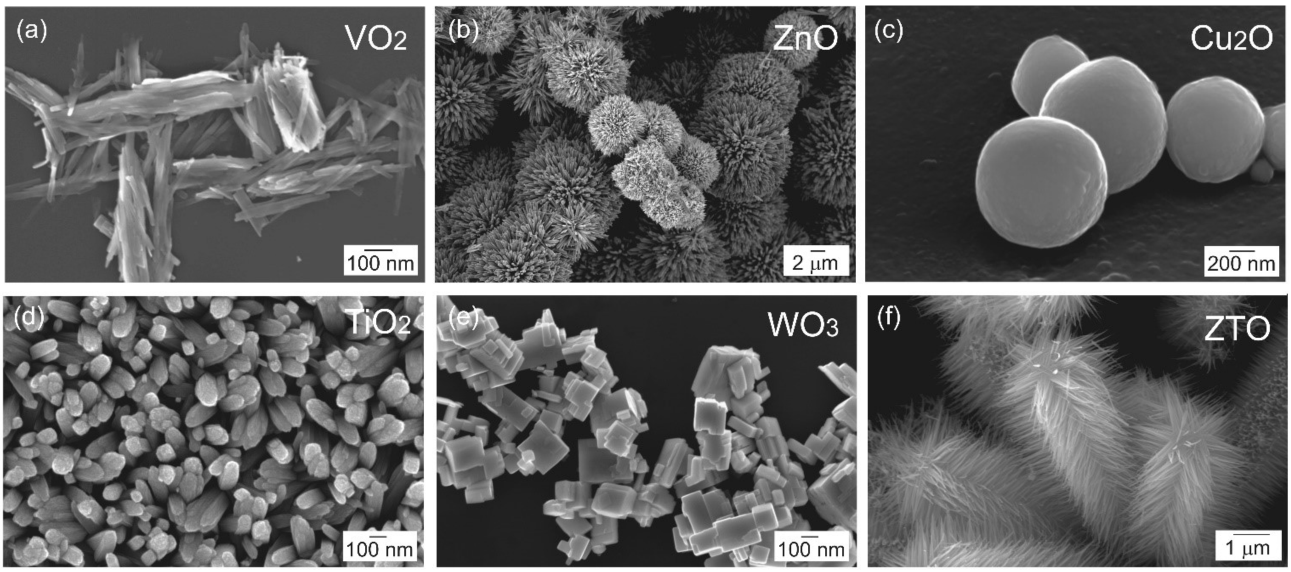

Fig. 1. SEM images of the metal-oxide nanostructures produced under microwave irradiation. (a) Vanadium oxide, (b) zinc oxide, (c) copper oxide, (d) titanium oxide, (e) tungsten oxide and (f) zinc-tin oxide.

Micro Moulded Interconnect Devices for Power Connector Applications

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Moulded Interconnect Device (MID) technology is well-established for application areas such as automotive, communications, biomedical and household electrical appliances, where electrical and mechanical functionalities are combined in a robust and cost efective way. MID are 3D injection moulded parts with integrated electrically conductive patterns on the surface. Amongst a number of processes, the conductive tracks can be created through the Laser Directed Structuring (LDS) method. During the procedure, the surface of the polymeric material is selectively activated by a laser in order to isolate the metal atoms from the organic ligands, allowing copper coating. Then, the mettalization on the activated area is obtained by the use of electroless plating (Fig. 1). The main advantages of LDS method in combination with 3D-MID technology are the reduction of the number of components in the final product since the mechanical and electrical functionalities are combined on the part, reduction of the number of assembly operations and the size of the final product.

The continued growth of micro applications also represents a big challenge for 3D-MID fabrication at the micro-scale. Production of LDS-MID requires special polymer materials, containing organic metallic complex particles, so that the laser can activate the circuit area and the metallization process can metallize only the engraving patterns. Nonetheless, the LDS method despite being one of the most industrially adaptive processes, it still requires integrated knowledge about materials, process conditions and product development.This work aims to study the influence of processing conditions of micro-parts, with different LDS-compatible materials, onto the quality of conductive tracks after sellective metallization process. This study will allow choosing the best processing conditions and material to fabricate a micro-3D-MID connector as case study.

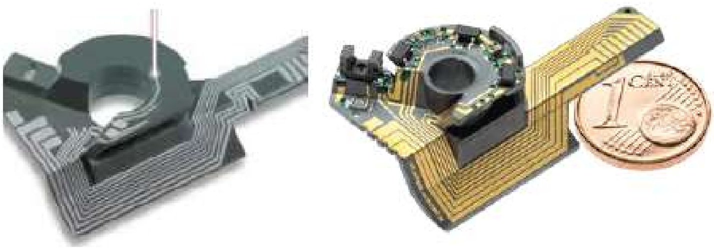

Fig. 1. Schematic of LDS process for 3D-MID fabrication.

Nonlinear optics in gas-filled kagomé microstructured optical fibres

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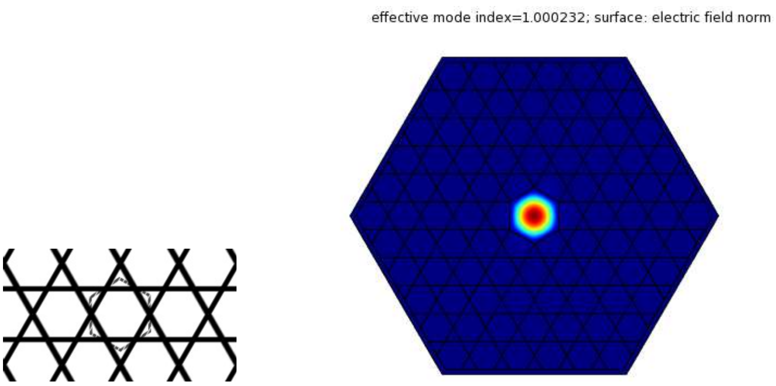
The microstructured optical fibres (MOFs), also called photonic crystal fibres (PCFs), are a novel class of optical fibres that have a microstructured design that runs the entire fibre length. They can be divided in two categories: solid-core MOFs which usually guide light by modified total internal reflection, and hollow-core MOFs which usually guide light by the photonic bandgap effect or other correlated effects. Amongst the HC-MOFs we have the kagomé fibres which allow the propagation of a broad wavelength range of light [1-2]. In this work we will study a kagomé fibre filled with different noble gases such as helium, argon, and xenon at various pressures. We will determine the group-velocity dispersion and the nonlinear parameter of those gas filled kagomé fibres. Then we will simulate the propagation of short pulses in the filled fibres that show high nonlinear parameter and good group-velocity dispersion profiles for generation of new wavelengths. The goal is to identify the parameters for which there is generation of UV light or supercontinuum light.



a) b)

Fig. 1. a) the unit cell of the cladding of a kagomé HC-PCF; b) the fundamental propagation mode of a kagomé HC-PCF filled with helium: core diameter dcore=40.0µm, thickness of the glass strands t=0.1µm, and gas pressure p=10.0bar, @λ=790nm.

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Optical fibre sensors in biomedical aplications

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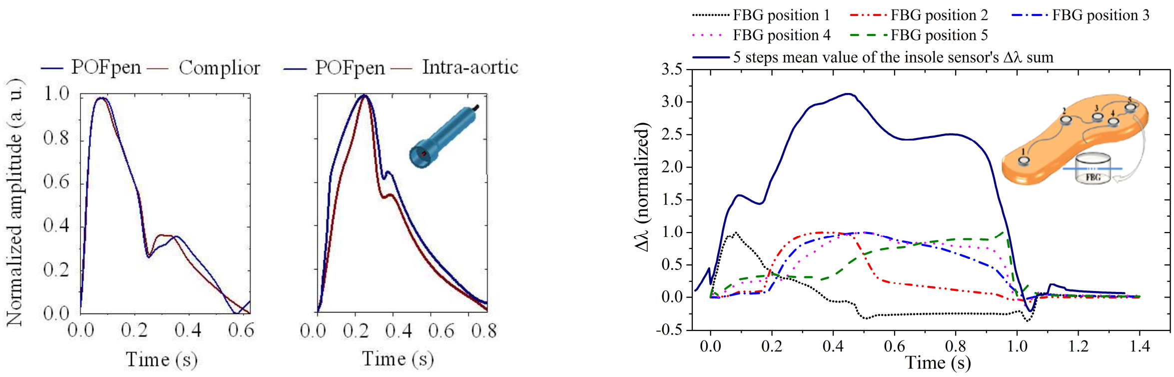
Optical fibre sensors have been developed for biomedical applications, namelly arterial cardiovascular wave pressure monitoring and physical rehabilitiation.

For the acquisition of the pulse wave in the carotid artery, towards its morphology analysis and central arterial pressure calculation, a low-cost intensity-based probe, POFpen, was developed and clinically tested [1, 2]. The sensor performance was compared to a non-invasive commercial device and to invasive catheterization testing. Preliminary results are shown in Fig. 1a).

In the physical rehabilitation field, a critical parameter to monitor is the foot plantar pressure, since it may indicate abnormal posture and other pathologies [3, 4]. We developed a new solution for plantar pressure monitor, consisting in a cork sole with 5 fibre Bragg grating (FBG) sensors incorporated in specific points of analysis, as shown in Fig. 1b).



a) b)

Fig. 1. a) Superimposed pulses assessed with POFpen, Complior and intra-aortic catheter. b) Cork sole with the incorporated FBG sensors, wavelength shift during gait and the sum of its values.

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Optimization of post-deposition annealing in Cu_2ZnSnS_4 thin film solar cells and its impact on device performance

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In this work we present an optimization of the post-deposition annealing, in Cu_2ZnSnS_4 (CZTS) thin film solar cells, applied at different stages of the solar cell preparation, namely, bare CZTS absorber, CZTS/CdS heterojunction and CZTS/CdS/i-ZnO/ITO complete solar cell. We performed current-density versus applied voltage measurements, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), Raman scattering, photoluminescence (PL) and X-ray photoelectron spectroscopy (XPS) studies to enlighten the mechanisms by which solar cells performance improvement comes about. As a result, we concluded that the optimum post-deposition annealing for CZTS is at 300 ºC for 15 mins and at atmospheric pressure. The highest efficiency gain was obtained when the absorber layer composition is close to the ideal one and when a single annealing step is performed on complete solar cells, where, we obtained efficiency improvements from below 1% to over 6.6%. Despite the observed improvement in device performance for annealing at intermediate stages it is, however, less pronounced than for full cell annealing. In this process we demonstrate cell performance improvements by a factor of 47. XRD results show a shift of all Bragg peaks to lower diffraction angle values, after post-deposition annealing. Also, the intensity of the peaks decreases and their full width at half maximum increases. PL measurements show that, post-deposition annealing, leads to a clear reduction of the nonradiative recombination channels and that the electronic structure is dominated by fluctuating potentials. XPS measurements reveal an interdiffusion of Cu, Zn and possibly Cd across the interface between buffer and CZTS absorber layers as the source of the significant observed cell performance enhancement.

Paper and Printed Electronics

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In this poster we present a glance of the concepts for paper-based electronic products developed at CENIMAT/I3N with potential application in a broad range of electronic commodities such as smart labels, intelligent packaging, or even foldable displays.

Part of the work being developed aims to explore paper and cellulose-based materials (vegetable and bacterial source) as dielectric material in transistors, memories or inverters, based oxide semiconductors and organic. On the other hand, cellulose based substrates are also being used for processing different electronic devices by simple and low cost techniques such as printing or even writing, resulting in printed/written transistors, memories, sensing elements or simple circuits, either by using paper as a substrate or by functionalizing it with conductor/semiconductor materials. The ultimate goal is to achieve low-cost, flexible and environmentally friendly and sustainable electronic devices, as demanded by modern society standards.

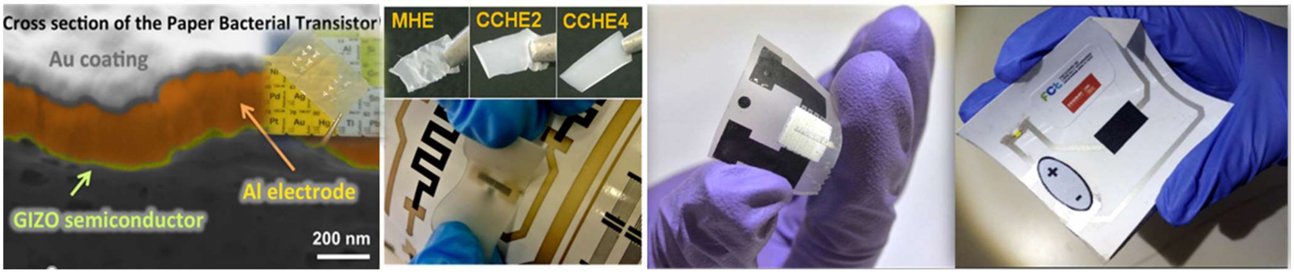

Fig. 1. Transistors and electronic circuits on cellulose-based substrates processed by PVD and printing techniques.

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Pauli limiting and metastability regions of superconducting graphene and intercalated graphite superconductors

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We present a study of metastability regions in the in-plane magnetic field *vs.* temperature phase diagram of graphene and intercalated graphite superconductors. Due to the vanishing density of states, undoped graphene requires a finite BCS interaction V_c to become superconducting (any finite doping drives this critical value to zero). Above V_c, superconducting graphene under in-plane magnetic field displays the conventional low temperature first-order transition (FOT) to the normal phase, but the width of the associated metastability region (normalized to the zero temperature critical field) vanishes when doping goes to zero and the interaction approaches V_c. In the case of intercalated graphite superconductors, modeled as two-dimensional two-band superconductors (a graphene-like band and a metallic interlayer band), a critical graphene intraband interaction is required in order for the appearance of a second metastability region in the superconducting region of the phase diagram. The width of this metastability region also goes to zero as the graphene intraband interaction approaches, from above, its critical value and the metastability region vanishes at the zero temperature supercooling field associated to the metallic interlayer band. Slightly above this critical value, the low-temperature FOT line bifurcates at an intermediate temperature into a FOT line and a second-order transition line.

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Performing controlled radical polymerization in the melt

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Polyolefins are often blended with other materials in order to improve their properties. However, the resulting composites lack from good phase compatibilization, which can be improved by the addition of compatibilizers or by preparing grafted copolymers.

"Grafting through", "grafting onto" and "grafting from" are examples of aproaches used for grafting macromolecules. Grafting from, in particular, is based on the polymerization of monomers using an already existing polymer as initiator. Among the polymerization approaches, controlled radical polymerization techniques [nitroxide-mediated polymerization (NMP), atom transfer radical polymerization (ATRP) or reversible addition−fragmentation chain-transfer polymerization (RAFT)] allow higher control over the structure and architecture of the produced polymers [1].

ATRP has been used to produce polymeric materials with different, well-defined, structures and architectures. Even though its high potential, it is commonly found in the literature reported at laboratory scale and performed in organic solvents. It would be of high interest if ATRP could be executed at industrial scale and without solvents.

Herein, we report the chemical modification of ethylene vinyl acetate (EVA) copolymer, adapting Moura *et al.* work [2], to produce, in the melt, an ATRP macroinitiator that can be used to develop polyolefins-based grafted copolymers (Fig. 1).

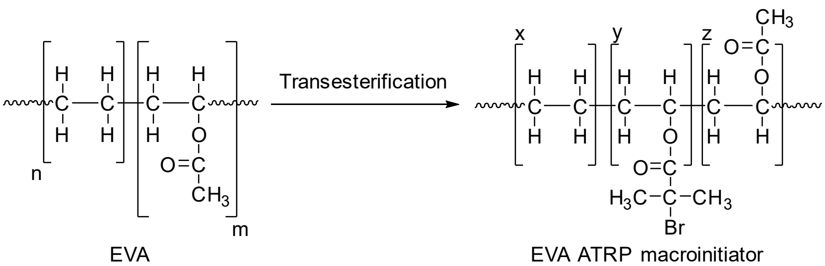

Fig. 1. Schematic synthetic pathway adopted for the preparation of the EVA ATRP macroinitiator.

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Photonic Nanostructures for Solar Cell Light Trapping with Colloidal Lithography

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Photonic structures, composed of a lossless but high refractive index dielectric material, are currently among the preferential solutions for light trappingin thin film solar cells; as they allow broadband manipulation of sunlight in order to strongly boost its absorptance in thin photovoltaic devices.

An innovative colloidal lithography nanofabrication method has been developed that allows the precise engineering of wavelength-sized features, with the materials and geometries appropriate for efficient light management when implemented on the front surface of solar cells.[1] This is a simple, low-cost and scalable approach presented here with TiO_2 nanostructures tested on amorphous-silicon absorber thin films coated on the rear side by a metallic reflector. The resultant array of wavelength-sized features acts as a nanostructured high-index anti-reflection coating, which not only suppresses the reflected light at short wavelengths but also increases the optical path length of longer wavelengths, via light scattering, within the absorber. The optical results have been compared with numerical electromagnetic computations to provide a deeper understanding of the physical mechanisms responsible for the absorptance enhancement in the cells. A notorious 27.3% enhancement in the cells photocurrent is anticipated with the fabricated structures, relative to conventional anti-reflection coatings.

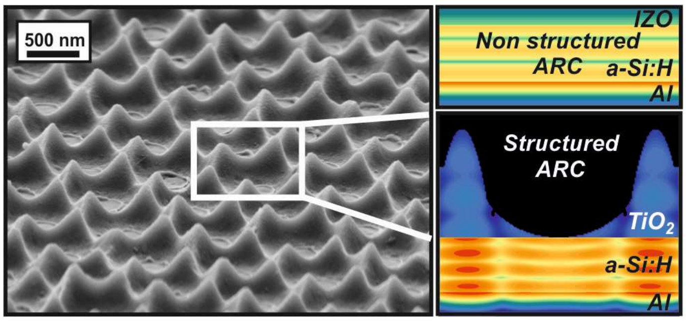

Fig. 1. *Left panel:* SEM of a the top view of a TiO_2 nanostructure. *Rigth panels:* FDTD computed log-scale distributions of the absorptance per unit volume, along cross-sectional planes of the structures with: IZO antireflection coating layer (upper panel) and with the nanostructure (bottom panel).

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Powerful recombination centers resulting from reactions of hydrogen with carbon-oxygen defects in solar silicon

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The introduction of Hydrogen has been shown to be an effective method to mitigate the recombination activity of several defects and impurities in solar Si. Nevertheless, we found that under certain conditions, Hydrogen atoms can interact with existing carbon and oxygen, resulting in the formation of powerful recombination centers [1]. Experimental data shows the formation of a dominant C-O-H related center with an acceptor level at E_v+0.36 eV. Here we propose a theoretical model, based on *ab-initio* calculations, that can be assigned to the experimental observation of the aforementioned recombination center. Our model consists in a bi-stable C-O-H defect with two distinct configurations in the neutral and negative charge state. The calculated reconfiguration barrier from the negative to the neutral state configuration is 0.22eV while the reverse path has virtually no barrier. This should allow for the defect to shift between configurations at room temperature upon capture of charge carriers. We predict an acceptor level for this defect at E_v+0.32 eV in good agreement with experimental observations.

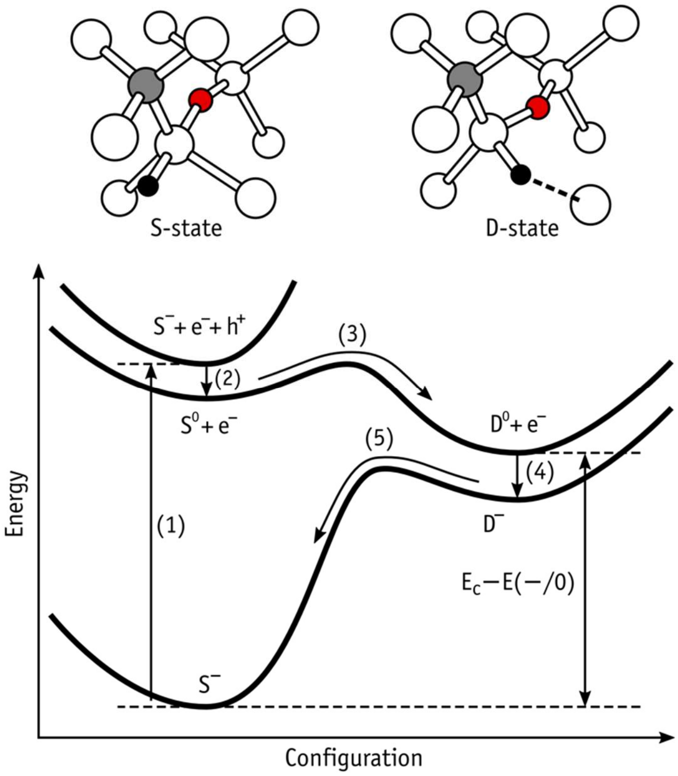

Fig. 1. Configuration-coordinate diagram of the model proposed to the minority carrier recombination mechanism in solar Si due to a C-O-H complex. C, O, H and Si atoms are shown in gray, red, black and white, respectively.

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Preparation, optical properties and temperature dependent upconversion luminescence of BBT:Nd glass upon 808 nm laser excitation

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This work reports on the preparation, optical properties and temperature dependent visible upconversion studies of neodymium doped bismuth barium tellurite (BBTNd) glasses prepared by melt-quench method. The phonon energy of the glass was estimated by Raman spectrum. Radiative parameters of various transitions/levels were calculated by applying Judd–Ofelt (J–O) theory. The concentration dependence of NIR emission and visible upconversion intensities of various levels has been discussed. Fig. 1 (a) and (b) show the upconversion bands in BBTNd glass when excited with 808 nm laser at different temperatures and (b) the energy level diagram representing the energy transfers and the subsequent transitions, respectively. Decrease of experimental lifetime of $^4F_{3/2}$ level with concentration has also been discussed by recording decay curves of the NIR emission and variation of upconversion spectral intensities with respect to sample temperature were studied.

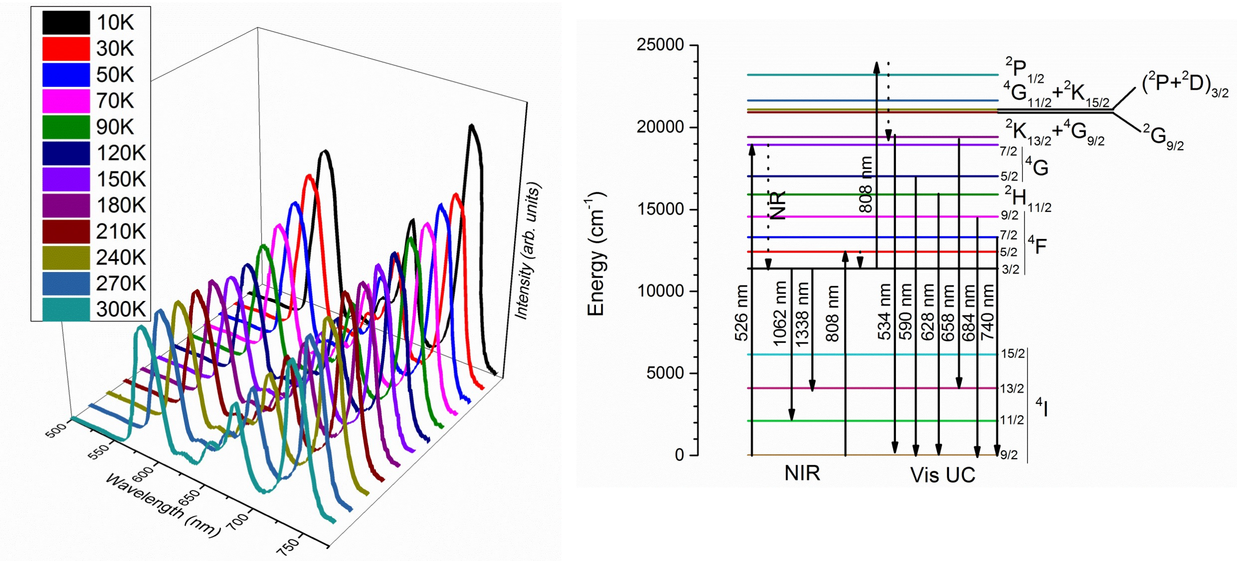

Fig. 1 (a) Temperature dependent visible upconversion and (b) energy level diagram of BBTNd glasses, respectively.

RHEOLOGY, A POWERFUL TOOL IN MATERIALS AND PRODUCTS CHARACTERIZATION

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In this work, a summary of the capabilities of performing rheological studies in CENIMAT, with reference to the equipment and possible measurements, is presented.

Examples of works performed by the group are shown:

- Rheological characterization of polymers
- Electrorheological study of liquid crystals: experimental and theoretical treatment.
- Rheology in optimisation of hydraulic grouts for masonry consolidation
- Electrorheology of hybrid inorganic/organic nanoparticles suspensions
- Real-time rheology of bacteria colonies

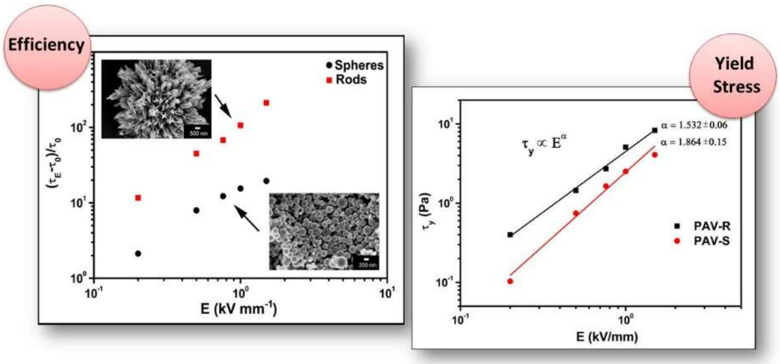

Fig. 1. Electrorheological behaviour of polyaniline-vanadium oxide nanostructures suspended in silicone oil: efficiency and yield stress in function of the electric field strength for two different particle shapes

Rheo-NMR study on the influence of ionic liquids in cellulose-based liquid crystalline solutions.

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Liquid crystalline cellulose-based solutions are at the origin of different kinds of multifunctional materials with unique characteristics that find application in photonics, microelectronics and soft stimuli responsive devices [1]. Ionic liquids (ILs) have become an important class of solvents over the past decades. These salts with melting points below 100 ºC have unique properties such as negligible vapour pressure, non-flammability, wide liquid range, high thermal and chemical stabilities, and high solvating capacities for inorganic, organic and polymeric compounds [2]. It is known that the cholesteric structure and lower critical solution temperature type phase-separation behaviour of lyotropic systems of cellulose-based solutions are significantly affected by the addition of a small amount of inorganic salts or ILs as the third component [3].

Herein we present our latest results on the study of liquid crystalline cellulosic solutions containing ILs using Rheo-NMR techniques. Combining deuterium NMR with rheology, we investigate the effect of imidazolium ionic liquids with different alkyl chain lengths on the cholesteric cellulosic liquid crystal system, under different shear rate regimes.

By adding a small amount of an imidazolium ionic liquid we drastically change both the flow and relaxation behaviour when compared with the anisotropic HPC-D_2O (50 wt.%) solutions.

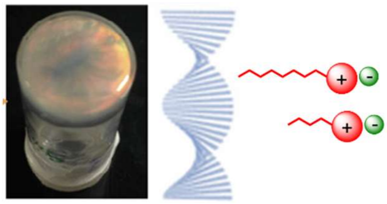

Fig. 1. HPC-D_2O/Ionic Liquid Solution

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Acknowledgements:

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SEM-EDS characterization of hard soldering with copper-tin alloy of Roman handle attachments from *Conimbriga* (Portugal)

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Hard soldering or brazing with Cu-Sn alloys applied to copper based artefacts has been used at least, since the Greek Period, although scarce studies have been made about their compositions. H. Lechtman and A. Steinberg [1] reported the rarity in finding hard soldering in ancient artefacts. Nevertheless, this kind of joining technique was important in Antiquity and should have been widely used during Roman times. Several solder vestiges were reported to be found in a collection of handle attachments of *situlae* from the archaeological site of *Conimbriga*, an important city in the Lusitania Province (Portugal) [2]. In the present work we are investigating the fusible metallic alloy present in 10 artefacts, which were cast in high leaded coppers and bronzes [3].

Scanning Electron Microscopy with Energy Dispersive X-Ray (SEM-EDS) microanalysis and Optical Microscope observations were made along the solder vestiges. Results point out to a standard composition around 60:40 wt.% of Cu:Sn, with Sn contents close to ε phase composition. Also, two features have been found a) melting of the interdendritic Pb-rich chains with long range diffusion of the solder alloy into the substrate and b) the etched surface of the solder/substrate interface showed an intermetallic phase (δ phase) resulting from high temperature Sn diffusion into the substrate.

Hard soldering alloys analysed exhibited rather homogeneous compositions in the opposite to the observed for the artefacts. These present rather diverse alloy compositions, apparently resulting from a poor control in the artefacts production [3]. Further studies should be made to better understand this process.

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SERS Substrates for Sensitive Molecular Detection

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Surface Enhanced Raman Spectroscopy (SERS) is a surface-sensitive technique that strongly enhances the Raman signal of molecules absorbed on the surface of metal nanoparticles.

At CENIMAT/i3N we are investigating the fabrication of silver nanoparticle (NP) plasmonic SERS surfaces grown by physical dewetting method and by chemical synthesis (in collaboration with the group of R. Franco, UCIBIO-FCT-NOVA and E. Pereira, ICETA-FCUP) on different types of substrates: silicon, glass, Tetrapack and paper.

The dewetting growth of Ag NPs on silicon and tetrapack substrates allows the formation of closed packed arrays of NPs with a controlled size of 60 nm that provides an enhancement of the Raman signal, designed by Enhancement Factor (EF) of up to 10^6, in a uniform and reproducible way [1]. On the other hand, paper substrates coated ZnO nanorods decorated with Ag NPs [2] (Fig. 1a) or with silver nanostars [3] (Fig. 2b) allows to obtain uniform SERS substrates with EF of 10^7, a state of the art results for paper SERS substrates.

A recent FCT funded project – DISERTOX aims to combine these SERS substrates with microfluidics to concentrate toxins and pesticides at the detection spot allowing to determine concentrations at sub ppb range, using low cost uniform efficient platforms.

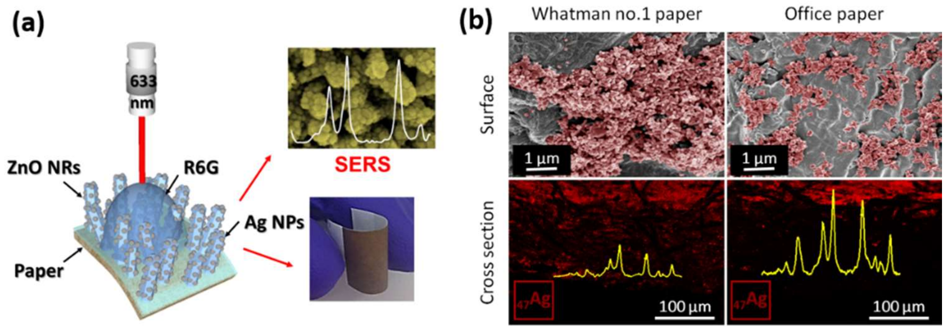

Fig. 1. (a) Scheme array of plasmonic ZnO nanorod forests on paper substrate for low-cost flexible 3D SERS, **(b)** SEM and EDS images of Ag NS on paper substrates.

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Shape Memory Alloys: from processing to applications

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Shape Memory alloys (SMA) are a class of functional materials with applications ranging from aeronautical to medicine. Their functional characteristics are strongly dependent on chemical composition and processing parameters, namely for the thermomechanical steps. At CENIMAT studies have been made on thermomechanical processing, welding and assessment of in service behavior, namely for applications in the field of orthodontics and endodontics. We will present an overview of studies on:

- Ni-Ti SMA alloys fabrication, from ingot casting to final thermomechanical processes, aiming to produce orthodontic archwires,

- assessment of shape memory effect and superelasticity on laser welded joints,

- assessment of functional characteristics of NiTi endodontic files and orthodontic archwires.

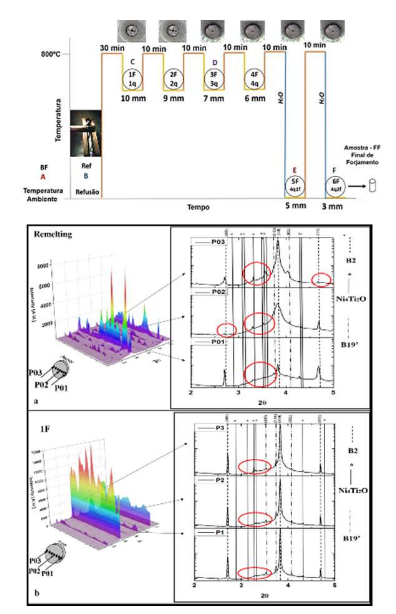

Fig. 1. Thermomechanical processing steps of Ni-Ti SMA.

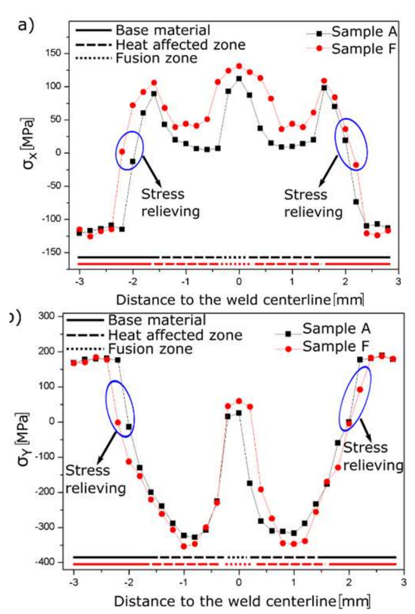

Fig. 2. Residual stresses on laser welded joints.

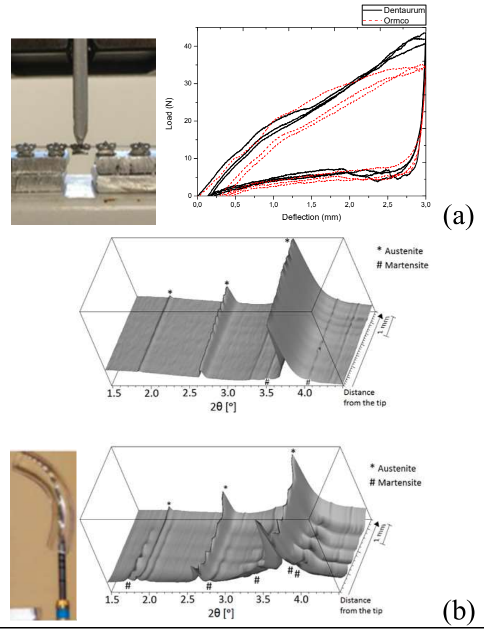

Fig. 3. (a) Bending test of orthodontic archwire. (b) Stress induced transformation on bent endodontic file (in situ SR-XRD).

SOLUTION BASED THIN FILM TRANSISTORS: FROM LAB TO FAB

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Amorphous metal oxides by solution processes have lately been used as an option to implement in flexible electronics, because it allows a reduction of the production costs. For that a substantial effort has been made to optimize both insulator and semiconductor layers in order to achieve enhanced performance/stability. This condition opens the possibility of moving from LAB to FAB processes.

This work aims to evaluate the progression from the simplest technique, spin-coating (Lab process) to inkjet printing (Fab process). Using spin-coating, great performance was achieved in indium–gallium–zinc-oxide (IGZO) TFTs with solution-based aluminum oxide (AlO_x) at low temperatures (150 °C) assisted by UV exposure [1]. In terms of semiconductors IGZO is the most widely used, due to its enhanced and stable electrical performance when compared with indium free metal oxides. Nonetheless, environmental demands require alternatives that rely on abundant and non-toxic elements. Zinc–tin-oxide (ZTO) is a good indium and gallium free alternative and promising results have been obtained with solution-based ZTO TFTs at 250 °C using spin-coating [2]. Precursor materials of AlO_x and ZTO were used to develop a suitable ink for inkjet printing and preliminary results at 350 °C were very promising. However our main focus is to reduce the annealing temperature, by combining thermal annealing with UV irradiation, to allow the process to be compatible with flexible electronics.

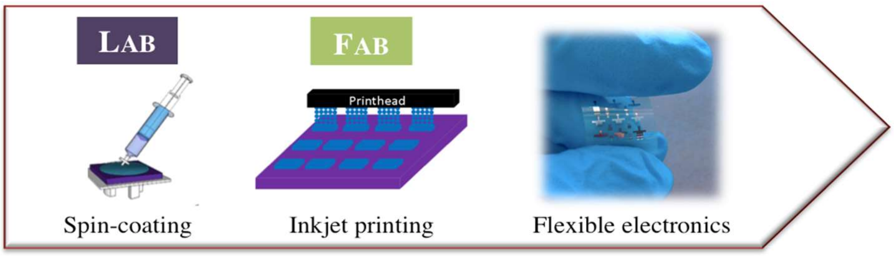

Figure 2. From Lab to Fab processes to produce flexible electronics.

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Space-division multiplexing in optical fibers

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Space-division multiplexing (SDM) has been proposed to increase capacity in fiber-optic communication systems [1]. SDM allows transmitting several parallel data streams through a single fiber using orthogonal modes of a few-mode fiber (FMF) or multiple cores in a multicore fiber (MCF). However, the cost-effectiveness of such solution will depend on the development of several compatible devices, e.g. spatial multiplexers, core/wavelength switches, or optical amplifiers, along with advanced digital signal processing (DSP) techniques for signal equalization after optical coherent detection.

We have demonstrated the viability of using Long Period Gratings (LPGs) in MCFs to develop different devices for multicore SDM [2, 3]. We theoretically demonstrated the use of LPGs to distribute a single pump source by all the cores of MCFs, and to promote the light transfer between the identical cores of heterogeneous multicore fibers producing inline selective core switching [2]. We demonstrated, experimentally, selective core coupling between two cores of a four-core fiber using LPGs, and successfully tested the device for a 200 Gb/s dual-polarization (DP) 16-quadrature amplitude modulation (16QAM) transmission signal [3].

In the digital domain, we have proposed space-demultiplexing algorithms based on signal analysis in higher-order Poincaré spheres for SDM transmission systems [4]. Such algorithms are modulation format agnostic and does not require training sequences. Using this approach, we have achieved signal demultiplexing for two modes/cores, with negligible signal-to-noise ratio (SNR) penalties for DP quadrature phase-shift keying (QPSK) and DP-16QAM constellations, and with a SNR penalty as lower as 0.5 dB for the DP-64QAM.

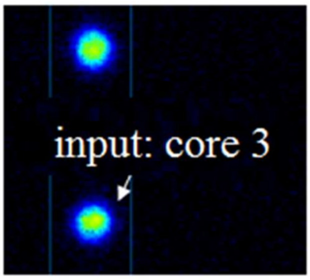

Fig. 1. Beam profiler images of the end-face of a 4-core fiber with a LPG inscribed, when a 1555 nm CW signal is injected into one core, showing the light transfer between core 3 and core 1 [3].

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Stabilization and accuracy improvements on a steady state viscoelastic computational code

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In this work we propose a methodology to improve the stability of the viscoelasticFluidFoam solver available in OpenFOAM®, aiming to increase the numerical stability and accuracy when dealing with viscoelastic fluid flows. The improvements are based on the modification of the discrete elastic-viscous stress splitting formulation that avoid the decoupling between velocity and stress fields. The accuracy enhancement is achieved using high-resolution schemes (MINMOD and SMART) to discretize the advection terms in the momentum and constitutive equations. The developments are assessed with two benchmark 2D case studies of an upper-convected Maxwell (UCM) fluid, namely the 4:1 planar contraction flow (41PC) and the flow around a confined cylinder (FACC), through the comparison with results available in the literature. In both cases, the simulations were performed at Re = 0.01, which correspond to creeping flow conditions, and Deborah number in range [0,5] and [0,0.8], respectively for the 41PC and FACC case studies. The results obtained in both test cases were accurately predicted in the sense that the vortex length size (41PC) and drag coefficient (FACC) were predicted with an accuracy of less than 0.6% and 0.08%, respectively, obtained by comparing the finest mesh result and the extrapolated value. In both case studies the method preserved the second order accuracy (see Fig. 1).

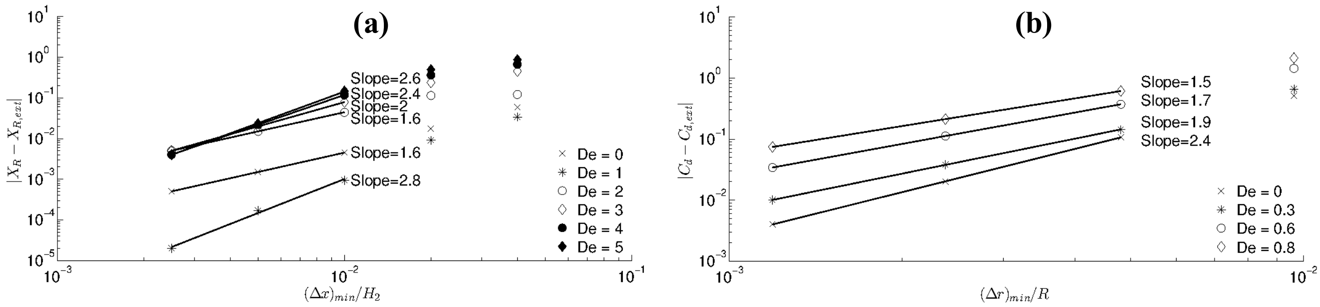

Fig. 1. Estimated error in (a) X_R and (b) C_d as a function of mesh refinement and De number for the UCM fluid in the 4:1 planar sudden contraction flow and flow around a confined cylinder case studies, respectively.

Stoneware microwave single-firing cycle

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Natural gas is the primary energy source in ceramic industries, the final firing stage representing up to 50% of the total energy costs. This work presents an alternative method for ceramic materials sintering using microwave radiation [1], a volumetric and more uniform heating process, with lower thermal gradients. Microwave heating can also enhance the densification rate, with more fine and more uniform grain structures, heading to better mechanical properties [2]. Heating rate of the microwave processing also affects the characteristics of different materials [2,3]. Results of macroscopic and microscopic studies on stoneware samples sintered conventionally (using an electric oven) and with microwave radiation are presented. The microwave sintered pieces require only one-half of the time (~70 min) and present a higher impact energy to crack compared with the gas sintered ones. Figure 1 presents the closed porosity fraction as function of the firing temperature, which is lower for the microwave sintered samples. For temperatures lower than 1050 °C it is observed a displacement of the microwave porosity curve to the left, and a convergence for temperatures higher than 1200 °C.

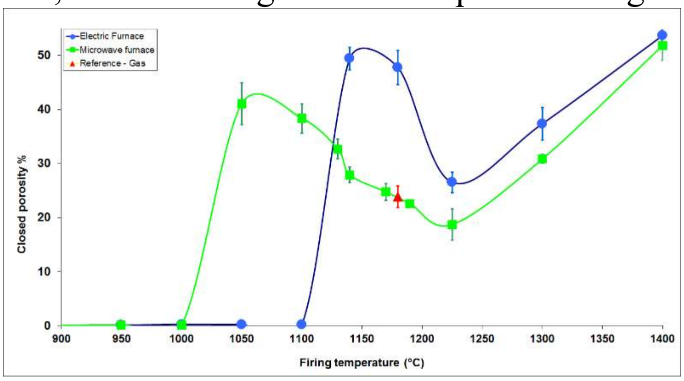

Fig. 1. Closed porosity of stoneware samples sintered using a conventional (electric) and the microwave heating technology.

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Sustainable Materials Based on Cellulose from Agro-Wastes

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Plastic materials produced from petrochemicals are used in a wide range of applications and most of them are extremely durable, requiring many years to degrade and, therefore became a significant source of environmental pollution [1]. To overcome this problem, several studies have been performed, aiming to search for new ecological materials toward innovative and cost-effective fabrication of bioplastics with similar performance to conventional ones [1,2]. Therefore, their development has become a key criteria for sustainable plastic production and consumption [2].

Bioplastics exhibit unique properties and can be produced from plants and crops wastes. Cellulose is a natural polymer derived from renewable resources, which offers the possibility to develop sustainable materials [2]. The present work aims to prepare new bioplastics based on extracted cellulose, from pumpkin peel agro-waste. Thus, the extracted cellulose was chemically modified to allow its dispersion in a polylactic acid (PLA) matrix. The resulting material was characterized in terms of its structural, morphological and thermal properties. This work showed the potential of food sector agro-wastes wastes as cellulose source, on the development of new bioplastics.

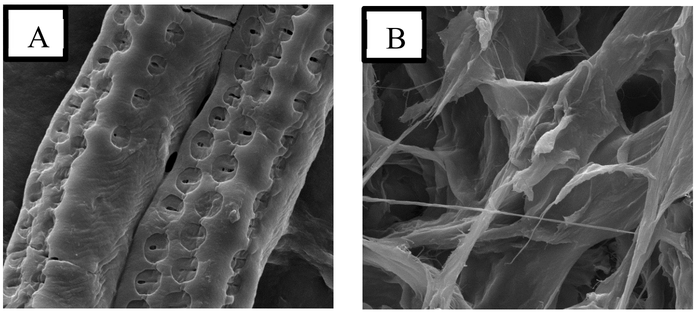

Fig. 1. SEM micrographs of raw pumpkin peel after dissolution in IL and precipitation (A) and chemically pretreated and dissolved in IL and precipitated (B).

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Synchronization in the random-field Kuramoto model on complex networks

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We study the impact of random pinning fields on the emergence of synchrony in the Kuramoto model on complete graphs and uncorrelated random complex networks. We consider random fields with uniformly distributed directions and homogeneous and heterogeneous (Gaussian) field magnitude distribution. In our analysis, we apply the Ott-Antonsen method and the annealed-network approximation to find the critical behavior of the order parameter. In the case of homogeneous fields, we find a tricritical point above which a second-order phase transition gives place to a first-order phase transition when the network is either fully connected or scale-free with the degree exponent $\gamma > 5$. Interestingly, for scale-free networks with $2 < \gamma < 5$, the phase transition is of second-order at any field magnitude, except for degree distributions with $\gamma = 3$ when the transition is of infinite order at $K_C = 0$ independent of the random fields. Contrary to the Ising model, even strong Gaussian random fields do not suppress the second-order phase transition in both complete graphs and scale-free networks, although the fields increase the critical coupling for $\gamma > 3$. Our simulations support these analytical results [1].

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Tailoring nitride semiconductor nanostructures towards optoelectronic nano-devices

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Group III-nitride semiconductors based on $Al_xGa_{1-x}N$ alloys span a wide range of bandgap energies that could enable the realization of laser diodes in the deep UV spectral range with interesting applications in the fields of bioagent detection, medical diagnostics, gas sensing, 3D printing and photolithography. For laser diode applications in particular, Favennec *et al.* [1] demonstrated that materials with wider bandgaps present lower thermal quenching of rare earth (RE) luminescence and higher efficiency induced by the RE-optical centers, enabling to explore the AlN-rich hosts such as AlGaN. In this work, europium (Eu)-implanted $Al_xGa_{1-x}N$ ($0 < x < 1$) nanostructures are deeply explored in order to tailor the material's original properties towards achieving high efficiency nano-devices. These nanostructures consist of *i)* $Al_{0.14}Ga_{0.86}N$/GaN short-period superlattices embedded in a diode structure grown by metal organic chemical vapour deposition on *c*-plane sapphire substrate, and *ii)* $Al_xGa_{1-x}N$ nanowires grown by molecular beam epitaxy on Si (111) substrate. The as-implanted nanostructures are further submitted to either rapid thermal annealing (RTA) or to high temperature and high pressure (HTHP) thermal annealing treatments in nitrogen in order to activate the Eu ions.

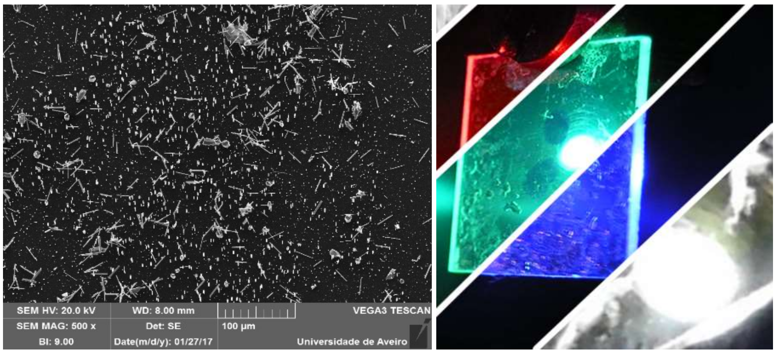

Fig. 1. *Left*: SEM image of Eu-doped GaN microwires. *Right*: Composed photographs of different GaN-based system emissions obtained by tailoring the bandgap and the structure. (the bright circle in the center corresponds to the saturation of the camera's detector due to the laser spot).

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TCAD simulation of oxide transistors

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In the past, Technology Computer-Aided Design (TCAD) tools for device simulation at a physical level proved to be a great asset for the development of silicon technologies. It is expected that the same root can be followed for oxide electronics [1] allowing for an understanding on how to further improve device performance and stability as required to meet the technology's full potential.

TCAD tools give insight on mechanisms behind device operation and allow for exploring different device configurations either in terms of their geometry or materials, accelerating the development process. In this work, Silvaco ATLAS^{TM} tool was used for simulation of indium-gallium-zinc oxide (IGZO) thin-film transistors (TFTs). Variations on the device's structure were explored, from scaling down the TFTs to submicron channel lengths to changing the overall architecture (e.g., from single to dual gate). Simulations for a dual-gate architecture can be seen in Fig.1 (a) where the effect of different biasing conditions for the second-gate is clear. In terms of material properties the effect of varying the density of states in the IGZO band-gap was investigated: Fig. 1 (b) shows simulations with increasing shallow donor-like states where the appearance of a "hump"-like behaviour in the transfer characteristics is observed [2].

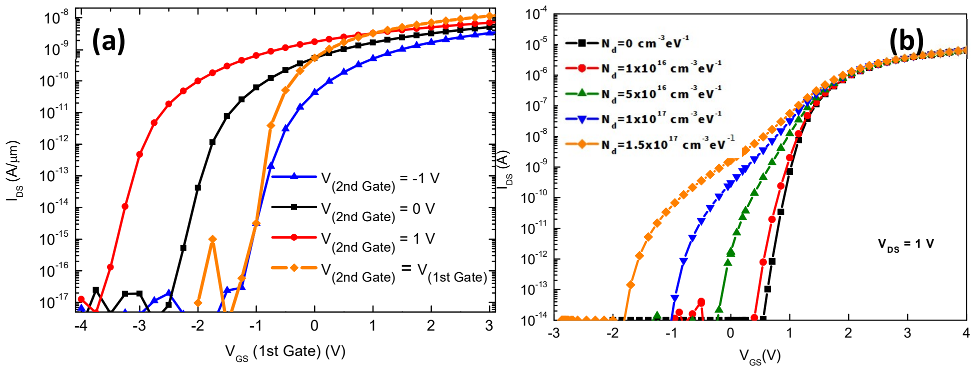

Fig. 1. (a) Transfer characteristics of dual-gate IGZO TFTs. **(b)** Increasing of hump-like behavior with concentration of shallow donor-like states.

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The use of additive manufacturing to fabricate microfluidic devices

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Currently, soft lithography is the most widely used technique to produce microfluidic devices with high geometric resolution and definition. However, this technique is largely constrained to planar structures and possibility to fabricate complex three dimensional features still remains a challenge. In this work we propose an alternative approach to produce microfluidic devices by means of PolyJet technology, which holds significant potential for single-step fabrication and enables enhanced control of the device geometry, such as complex 3D flow paths with non-standard cross sections. PolyJet is the trademark given by *Stratasys* (Eden Prairie, MN, USA) to designate their own line of 3D printing machines based on layer-by-layer deposition of UV photocurable polymer. Among other 3D printing methods (e.g., FDM, SLS, SLA), this technology employs the highest layer resolution (approximately 16µm) enabling the production of highly accurate, smooth and detailed models. Here we present some examples of microdevices produced by this technology.

Topological two-body states in SSH chains with interactions

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We address the effect of nearest-neighbor (NN) interactions on the topological properties of the Su-Schrieffer-Heeger (SSH) chain, with alternating hopping amplitudes t_1 and t_2 [1]. Both numerically and analytically, we show that the presence of interactions induces phase transitions between topologically different regimes. In the particular case of one-hole excitations in a half-filled SSH chain, the V/t_2 *vs.* t_1/t_2 phase diagram has topological phases at diagonal regions of the phase plane. The interaction acts in this case as a passivation potential. For general filling of the SSH chain, different eigensubspaces of the SSH Hamiltonian may be classified as topologically trivial and non-trivial. The two-hole case is studied in detail in the large interaction limit, and we show that a mapping can be constructed of the two hole SSH eigensubspaces into one-particle states of a non-interacting one dimensional tight-binding model, with interfaces between regions with different hopping constants and local potentials. The presence of edge states of topological origin in the equivalent chain can be readily identified, as well as their correspondence to the original two-hole states. Of these states only some, identified by us, are protected and, therefore, truly topological. Furthermore, we found that the presence of the NN interaction generates a state where two holes occupy two consecutive edge states. Such many-body states should also occur for arbitrary filling leading to the possibility of a macroscopic hole gathering at the surface (at consecutive edge states).

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Tuning cellulose nanocrystal films photonic properties

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Iridescent solid films with periodic helicoidal structures that reflect only left circularly polarized light, can result from drying cellulose nanocrystals liquid crystalline water suspensions [1]. Here we report the use of solid cellulose nanocrystals iridescent films to produce a new photonic structure, which reflects both right and left circular polarizations. The effect originates from the infiltration of a nematic liquid crystal layer in micrometric sized planar gaps existing perpendicular to the cross section of the solid film, between the two left-handed cellulose nanocrystals cholesteric domains with different pitches. The anisotropic layer acts as a half-wave phase retarder. Furthermore, one can reversibly tune the photonic properties of cellulose nano composites by application of an electric field or temperature variation, by changing the birefringence of the liquid crystal layer [2]. This work paves the way to the usage of cellulose nanorods iridescent films to new photonic applications as, for example, tunable reversible reflective displays.

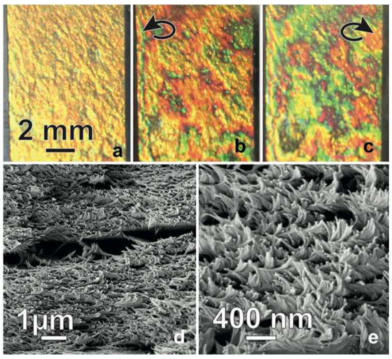

Fig. 1. Photographs of CNC and 5CB composite film observed through a) unpolarised white light and circularly polarized light showing different colour reflection in a) LCP and b) RCP light channels. d) SEM image of a film's cross-section where a micro-gap is visible and in e) one can see the cholesteric arrangement of CNC within the film's structure. [2]

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ZnO nanostructures and applications

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ZnO is a promising multifunctional, n-type semiconductor material, with a wide and direct band gap of about 3.37 eV and a large free exciton binding energy of 60 meV at room temperature which allows it to act as an efficient semiconductor material. Is biocompatible and also displays piezoelectric properties. Due to these different properties, ZnO is used in various bio, micro and nano electronic applications, such as thin film transistors, dye-sensitized solar cells, UV/ozone sensors, piezoelectric devices, photocatalisis, SERS, glucose sensor and in biomedical science as antibacterial and antifungal agents [1]–[3].

For this propose, different growth techniques, precursors and solvents are continuous being employed to prepare a variety of different ZnO nanostructures, like chemical vapour deposition, electrodeposition, electrospinning, LAFD (laser assisted flow deposition) and hydrothermal method, whether by conventional heating or assisted by microwave radiation.

With this work ZnO nanostructures are synthesized in few minutes. It will be shown how, by using different types of substrates, this material can be use in different applications

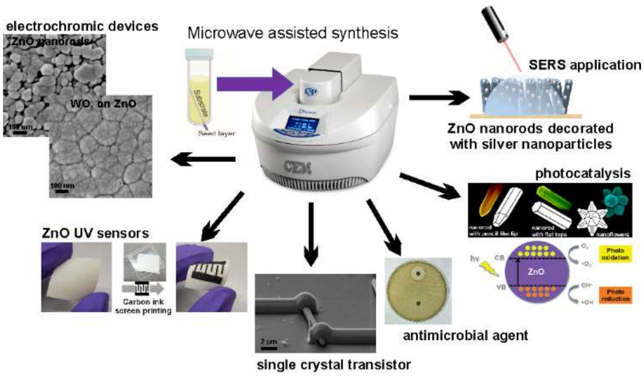

Fig. 1. Esquematic of ZnO nanoparticles applications

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