INSTITUTE FOR NANOSTRUCTURES, NANOMODELLING AND NANOFABRICATION

RESEARCH, INNOVATION AND ENGINEERING APPLICATIONS

VIII Annual Meeting

03-04 March 2023

Leiria, Portugal

INSTITUTE FOR NANOSTRUCTURES, NANOMODELLING AND NANOFABRICATION

NOVA SCHOOL OF SCIENCE & TECHNOLOGY

universidade de aveiro

Front cover: STEM image taken by Daniela Gomes and edited by Paula Soares

PROGRAM AND ABSTRACT BOOKLET

VIII ANNUAL MEETING i3N 2023

Eurostar Leiria & Jardim Hotel, Leiria

03-04 March, 2023

Organization committee: Paula I. P. Soares, Henrique Vazão Almeida

ACKNOWLEDGEMENTS

VIII Annual Meeting i3N

03-04 March 2023

Leiria, Portugal

This meeting is funded by National Funds through the FCT - Fundação para a Ciência e a Tecnologia, I.P., under the scope of the projects UID/50025/2020-2023 and LA/0037/2020.

fct Fundação para a Ciência e a Tecnologia

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ABOUT THE MEETING

The Institute for Nanostructures, Nanomodelling and Nanofabrication (i3N, https://www.i3n.org/), with two hubs, one in Aveiro and the other in Caparica (https://www.cenimat.fct.unl.pt/) promotes every year a scientific journey to identify the outcomes reached by the different groups that constitute i3N, along 4 key thematic lines:

- Sustainable Micro and Nanofabrication;
- Green and Clean Energy Systems;
- Nanomaterials Engineering and Functional Interfaces;
- Biomedical Devices and Systems.

Besides that, we discuss the strategy and new challenges we have along the research pathway we expect to impact on knowledge and generate innovation.

The organization committee would like to thank the keynote speakers, Professor Aline Rougier and Professor Pable Ordejón, and the plenary speaker, Professor Juan Ramón Morante.

This year we organize our event in Leiria, at the Hotel Eurosol, Leiria & Jardim Hotel, from 3-4 March 2023.

PROGRAM

Friday, 03rd March 2023	
11h00-11h45	**Registration**
11h45-12h30	**Opening Ceremony** i3N Director, Full Professor Rodrigo Martins NOVA Rector, Full Professor João Sàágua (To designate) Aveiro Rector, Full Professor Paulo Jorge Ferreira (To be confirmed) FCT NOVA Dean, Full Professor José Alferes (To be confirmed) i3N Aveiro Pole, Professor Florinda Costa
12h30-14h00	**Lunch**
14h00-14h30	**Keynote Talk – Professor Aline Rougier** Senior CNRS Researcher, Institute of Condensed Matter Chemistry of Bordeaux (ICMCB), Bordeaux University, France "Powder and thin films for optimized chromogenic properties" - (25 mins+5)
14h30-16h00	**Presentations Groups Responsibles** (12 mins each presentation +3 mins) - Advanced Functional Materials for Micro and Nanotechnologies (AFMMN)- FCT NOVA - Physics of Advanced Materials and Devices (PAMD) - Aveiro - Soft and Biofunctional Materials Group (SBMG) - FCT NOVA - Theoretical and Computational Physics (TCP) - Aveiro - Structural Materials (SM) - FCT NOVA - Nanophotonics and Optoelectronics (NO) - Aveiro
16h00-17h45	**Posters Session/Coffee break**
17h45-18h15	**Keynote Talk – Professor Pablo Ordejón** Director of the ICN2 - Institut Català de Nanociència i Nanotecnologia - (25 mins+5)
18h15-19h00	**Presentations Thematic Lines** TL1 - Sustainable Micro and Nanofabrication – FCT NOVA TL2 - Green and Clean Energy Systems – FCT NOVA TL3 - Nanomaterials Engineering and Functional Interfaces - Aveiro TL4 - Biomedical Devices and Systems - Aveiro (8mins+2)
19h00-20h00	**Meeting with EAB and SIC** (Director, Executive Board, Research Group Leaders (RGL), Thematic Lines Coordinators (TLC), External Advisory Group (EAB) and Strategic Innovation Council (SIC))
20h00	**Dinner (<u>Location</u>: <u>Quinta do Paul</u>)** **(Oral Interventions from External Advisory Group (EAB), Strategic Innovation Council (SIC) and Announcements)** **Awards:** - i3N Publications with the highest Impact Factor 2021-2022, for Pole Aveiro and other for Pole FCT NOVA - Best Poster for Pole Aveiro and other for Pole FCT NOVA
Saturday, 04th March 2023	
08h45-09h30	**Plenary Talk – Professor Juan Ramón Morante** Director Catalonia Institute for Energy Research (IREC) "Catalyst for a renewable driven circular economy and energy transition" - (40 mins+5)
09h30-10h15	**Presentations PhD Students Aveiro and FCT NOVA** Groups AFMMN/ PAMD/ NO - (12 mins each presentation +3 mins)
10h15-10h30	**Coffee break**
10h30-11h15	**Presentations PhD Students Aveiro and FCT NOVA** Groups SBMG / TCP/ SM - (12 mins each presentation +3 mins)
11h15-12h45	**General Meeting - Summary Conclusion**
12h45-13h00	**Concluding remarks and closing** Minister of Science, Technology and Higher Education, Professor Elvira Fortunato
13h00	**Lunch**

Detailed Orals

Friday, 03 March 2023		
14h30-16h00	**Presentations Groups Responsibles** (12 mins each presentation +3 mins)	
Group	**Responsible**	**Pole**
Advanced Functional Materials for Micro and Nanotechnologies (AFMMN)	Pedro Barquinha	FCT NOVA
Physics of Advanced Materials and Devices (PAMD)	Luís Cadillon Costa	Aveiro
Soft and Biofunctional Materials Group (SBMG)	João Paulo Borges	FCT NOVA
Theoretical and Computational Physics (TCP)	António Ferreira	Aveiro
Structural Materials (SM)	João Pedro Veiga	FCT NOVA
Nanophotonics and Optoelectronics (NO)	Paulo Antunes	Aveiro

18h15-19h00	**Thematic Lines** (8mins+2)	
Thematic Line	**Responsible**	**Pole**
TL1 - Sustainable Micro and Nanofabrication	Rodrigo Martins	FCT NOVA
TL2 - Green and Clean Energy Systems	Manuel Mendes	FCT NOVA
TL3 - Nanomaterials Engineering and Functional Interfaces	Luiz Pereira	Aveiro
TL4 - Biomedical Devices and Systems	João Veloso	Aveiro

Saturday, 04 March 2023	
09h30-10h15	**Presentations PhD Students Aveiro and FCT NOVA Groups** AFMMN - Tomás Pinheiro PAMD - José Cardoso NO - Ana Isabel Freitas (12 mins each presentation +3 mins)
10h30-11h15	**Presentations PhD Students Aveiro and FCT NOVA Groups** SBMG - Catarina Chaparro TCP - Filipe Barroso SM - João Cardoso (12 mins each presentation +3 mins)

GENERAL INFORMATION

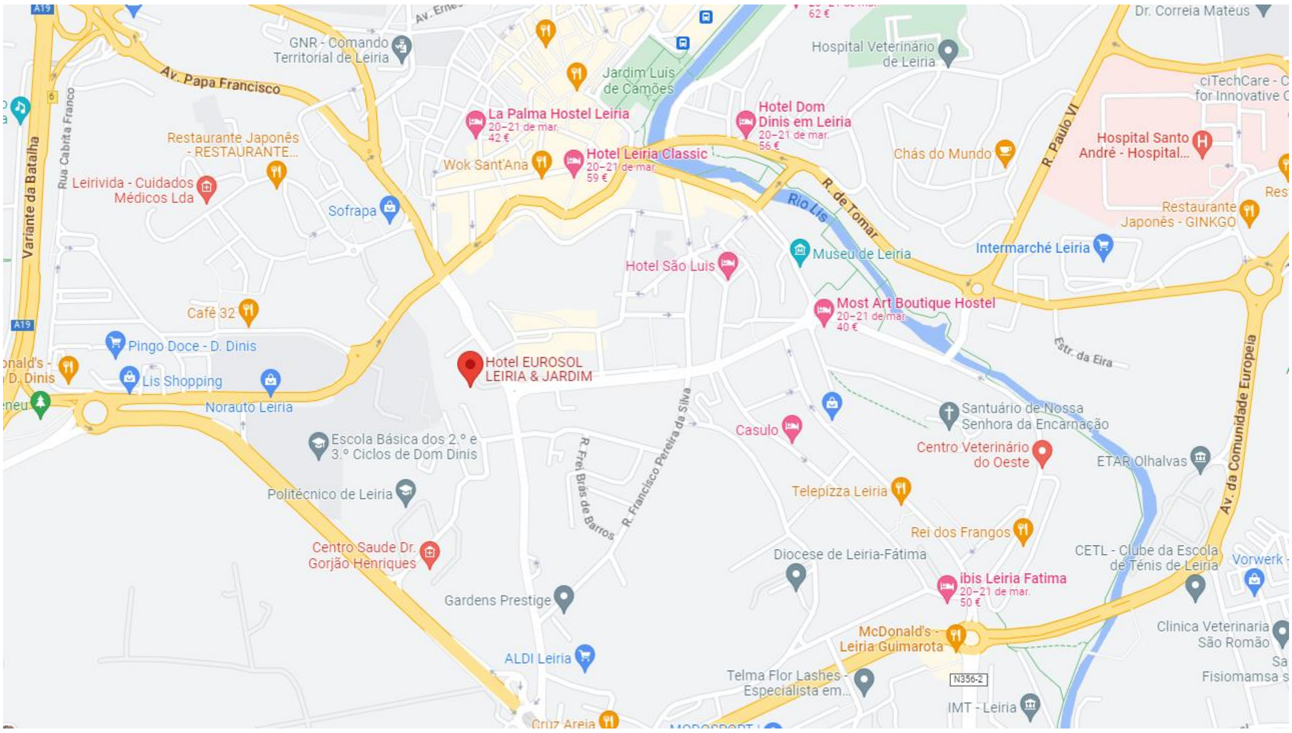
Conference Venue

Eurosol Leiria & Jardim

Rua D. José Alves Correia da Silva

2410-117 - Leiria

Portugal



GENERAL INFORMATION

About Leiria

Leiria is a city located in central Portugal, in the district of Leiria. It is the capital of the Leiria municipality and has a population of approximately 130,000 people. Leiria is a historic city, dating back to the Roman era. It has a rich cultural heritage and is home to several historic landmarks and monuments, including the Leiria Castle. In addition to its historical and cultural attractions, Leiria is also known for its vibrant arts and music scene. It hosts several festivals and events throughout the year. The city is surrounded by natural beauty, including the Serra de Aire e Candeeiros Natural Park, which is a protected area known for its rugged limestone landscape, caves, and underground rivers. The nearby beaches of Nazaré are also popular spots for surfing. Overall, Leiria is a charming and lively city with much to offer visitors and residents alike, from its rich history and culture to its stunning natural surroundings and vibrant arts scene. For Dom Afonso Henriques, the first Christian conqueror of Leiria in 1135 and the founder of its castle, the town was the advance guard for his strategy of conquering Sintra and Lisbon from the Moors, which took place in 1147. In the 14th century, Dom Dinis resided in the castle on several occasions. The king's reign was particularly marked by the planting of the Leiria pine-forest all along the coastal strip in order to protect the sand dunes from erosion. Its maritime pines were to provide the timber and pitch used in the building of Portuguese ships, especially during the period of the Discoveries. The city spread outside the walls of its mediaeval castle, the first phase of its growth being marked by the building of the Romanesque Igreja de São Pedro, followed by the building of the cathedral and the Igreja da Misericórdia in the 16th century. The city then spread all the way down to the river Lis and various religious buildings were built on its tree-lined banks. (from: www.visitportugal.com)

GENERAL INFORMATION

NOVA School of Science and Technology (NOVA FCT)

The NOVA School of Science and Technology (FCT NOVA) is one of the three largest and most prestigious schools of Engineering and Sciences in Portugal. It is located 15 minutes away from Lisbon, is renowned for its excellence in research, for the quality of its courses and for the large employability of its graduates (graduates, masters, doctors).

FCT NOVA, with about 8000 students, it has one of the best university campuses and is distinguished by a culture of excellent teacher-student relationship and an intense academic life with many different cultural and sport activities.

All courses are accredited by the A3ES (Agency for Assessment and Accreditation of Higher Education) and all Engineering courses are recognized by the Order of Engineers, FEANI (Federation of Professional Engineers that unites national engineering associations from 33 European Higher Education Area (EHEA) countries) and EUR-ACE (European Accredited Engineer).

FCT NOVA is structured in 13 Departments and 16 Research Centers, offering 102 study cycles (18 Bachelor's, 11 Integrated Master's (no applications available for the academic year 2021/2022), 41 Master's and 32 PhDs).

Its scientific production, resulting from the publication of a large number of articles in international scientific journals of great demand and quality, gives it wide international recognition (the value of the scientific production index - SciVal Citation Impact - is 1.35, FCT NOVA is 35% above the world average). This performance allows the Faculty to integrate the main technological university networks, such as the CESAER network and to participate in consortiums with European and US universities, namely MIT, CMU and the University of Texas.

The participation in 9 COLABs and the 14 ERC scholarships obtained by FCT NOVA researchers (the largest concentration of these laboratories and scholarships in Portuguese Universities), demonstrates how the NOVA School of Science and Technology is oriented towards the future and based on vanguard international research.

NOVA SCHOOL OF SCIENCE & TECHNOLOGY

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

GENERAL INFORMATION

University of Aveiro

The University of Aveiro (UA) is a public foundation under private law whose mission is to contribute to and develop graduate and postgraduate education and training, research and cooperation with society. The University of Aveiro (UA) was founded in 1973 and paved the way in the creation of teaching offers in several knowledge fields. Today, UA is widely recognised as one of the most innovative universities in Portugal, the quality of its teaching and research and for its cooperation with regional and national business.

Its organization and matrix structure, encompassing University and Polytechnic subsystems, stimulates knowledge exchange and cross-contamination between knowledge fields, promoting a useful proximity between teaching and research, which results in a very appealing message for national and international students.

With a modern and prestigious architecture, UA occupies top positions in the most important international rankings that assess Higher Education institutions.

The UA is therefore made up of organisational units within the university sub-system (16 departments) and the polytechnic sub-system (four schools), which include the teachers responsible for teaching their courses. An integral part of the university's structure are a set of units dedicated to various research activities, and within the framework of the third university mission (cooperation with society), there are interface structures that establish links with the both the local region and society as a whole.

The University is also equipped with common governing and global management entities responsible for scientific and pedagogical functions, as well as unit-level organizations and other hierarchical structures. Equally, a fundamental part and parcel of the organization are a series of services run by the university's administrative services which embrace the overall activity of the institution.

universidade de aveiro

https://www.ua.pt/

GENERAL INFORMATION

I3N

Created in 2006 as Associate Laboratory by the Portuguese Minister of Science, Technology and Higher Education. i3N is a partnership between 2 leading research units in fundamental and applied science: CENIMAT (Materials Research Center, NOVA University of Lisbon) and FSCOSD (Physics of Semiconductors, Optoelectronics and Disordered Systems, U. Aveiro). Since 2018 i3N follows a strategic refocus of the main scientific activities in advanced functional materials/devices for nanosciences and nanotechnologies.

i3N researchers have achieved excellent scientific results that have been recognized with the award of 6 ERCs grants as well as the number of international projects and patents along the scientific papers published at high impact factor journals, like Science, Nature, Progress in Materials Science and Advanced Materials, which places i3N as the leading research institute in Portugal in the area of Materials Science and Nanotechnologies.

During the last years, i3N has consolidated its strategic research activity in order to overcome the innovation challenges associated to Nanotechnologies, Nanomaterials and Nanosciences in accordance with the policies established by Horizon 2020 (and now to be implemented with FP9), with the purpose of improving the level of materials science and technology understanding and their use as enabler to serve multi-sector applications.

We believe that the combined strengths of a collaborative team are by far, orders of magnitude larger than the sum of the individuals. Nanoscience and Nanotechnology in strong relation with Advanced Functional Materials are the front of modern research. The fast-growing economy here requires experts with outstanding knowledge in these areas in combination with the skills to apply it in new products. At i3N we are also training the future generations for academia an industry.

Invited speakers

PLENARY SPEAKER

Joan Ramón Morante Lleonart

Director Catalonia Institute for Energy Research (IREC)

Professor J.R. Morante has been full professor at the Faculty of Physics at the University of Barcelona since 1985. Since 2009 he has been director of the area of advanced materials for energy at the Institute for Energy Research of Catalonia, IREC, and since the end of 2015 he has been director of this public research institute. https://www.irec.cat/

He has previously been Vice Dean and Dean of the Faculty of Physics at the University of Barcelona, director of the Department of Electronics at this university, head of studies in Electronic Engineering and also he was co-coordinator of the University of Barcelona and Polytechnic University of Catalonia interuniversity master's degree on Energy.

Currently, his activities focus on the introduction of renewable energies and the environmental impact of energy. Likewise, he is involved in the deployment of new energy carriers such as hydrogen, biomethane or synthetic fuels for a sustainable mobility, a decarbonized industry, cities, and societies.

He has co-authored more than 600 publications with more than 36.000 citations (GS) with h factor 103. He has 24 patents, has been director of 56 doctoral theses, has participated/coordinated in numerous projects of different international and industrial programs (> 60) and has been distinguished with the Narcís Monturiol medal from the Generalitat de Catalunya. He is currently president of the European Materials Society.

Presentation ID: PL1 Type of Presentation: Oral

Catalyst for a renewable driven circular economy and energy transition

J. R. Morante[1]*

[1] IREC Jardins de les Dones de Negre,1. Sant Adrià del Besòs 08930. Spain; University of Barcelona, C/ Martí Franquès 1, Barcelona 08028. Spain

The great challenge for humanity to face climate change and the depletion of resources is the substitution of fossil sources used to produce energy and to obtain products that today are still obtained from oil.

Only with this substitution can a circular economy be started that optimizes the use of resources and ensures the sustainability of the planet. Therefore, renewable sources become the motor of the new forms of circular economy and, at the same time, determine the energy transition to meet the requirements to achieve the electrification and/or decarbonization of our society, without CO_2 emissions. For this, the rational development of the catalysts becomes a fundamental key. It is necessary to have highly effective and appropriate catalyst materials to efficiently generate energy, store energy with high round-trip efficiencies, or give rise to reactions to obtain new energy vectors or value-added chemical products that make petrochemical industrial production sustainable or promote the recovery of waste or the bioenergy production.

In this scenario, for achieving rational design of catalyst, the nanoreactor concept becomes a significant contribution. Nanoreactors in a general sense are considered as structures of materials defined at the nano level scale with a nucleus space and the ability to link one or more molecules guests just to achieve different functionalities. So, confined space within a nanoreactor increases the concentration of reactants and can effectively influence the reaction rate through binding interactions with the linked molecules controlling multi-steps catalytic reactions.

These features play a significant role concerning to oxidation and reduction reactions needed in many energy systems like batteries o electrochemical cells such as those used for CO_2 or nitrates reductions as new green alternative processes.

In this contribution we will be focused on examples for sustainable chemistry and more eco-efficient chemical syntheses routes. The reported nanoreactor examples facilitate safer and more energy-efficient production routes, higher-yield, cleaner and more resource-efficient synthesis of large volumes of chemicals: reduction of CO_2, reduction of nitrate and application in Lithium Sulphur Battery, LSB, will be assessed and discussed, showing with these examples the advantages in the use of this approach. It demonstrates that the integration between nanoreactor and catalysis is thus a key factor towards scientific and technological breakthrough in electrochemical or synthesis processes for a sustainable energy systems.

KEYNOTE SPEAKER

Aline Rougier

Directeur de Recherche CNRS ICMCB, Bordeaux, France

Dr. Aline Rougier received her PhD from University of Bordeaux in Solid State Chemistry and Materials Sciences. CNRS researcher since 1998, her work in the field of inorganic materials for energy storage and energy conversion applications has been mainly focused on oxides and thin films looking at the relationship between the materials structure, composition, morphology and their properties. Her main topic concerns more specifically the study and optimization of electrochromic materials as powders or thin films, from deep investigation of their optical and electrochemical properties to their integration in devices for applications in the visible and the infrared regions. In the past few years, she extended her activities to thermochromism. Since 2011, she is the editor in charge of papers for the international scientific journal Solar Energy Materials and Solar Cells, expert in “optical and electrical properties” handling about 200 papers per year. She has authored 180 papers in the field of materials for energy and had co-organized close to 20 international symposia.

Presentation ID: KN1 *Type of Presentation: Oral*

Powder and thin films for optimized chromogenic properties

A. Rougier[1,2]*

[1] *CNRS, ICMCB, UPR 9048, 87 avenue du Dr Albert Schweitzer, F-33608 Pessac, France; 2 Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France*

Chromogenic materials exhibit tunable properties as a consequence of an external stimulus such as light (photochromism), temperature (thermochromism) or potential (electrochromism). Those smart compounds find applications in buildings and automobile industry by controlling light and heat transfer through windows for transmissive devices while colour changes in reflective devices offer great interest in the field of displays and printed electronics. In this presentation, through various examples, we will illustrate the key role played by the synthesis or/and the deposition route on the physico-chemical properties of mostly oxides powders and thin films as well as on their chromogenic properties. In particular, multichromism, namely thermochromism and electrochromism, in vanadium oxides will be discussed in respect of the oxide stoichiometry. Beside the influence of shaping in form of nanopowders synthesized through the polyol process [1] or of thin films of few hundred nanometers grown by RF sputtering method or thick films of few micrometers by doctor blading on the chromogenic properties will be illustrated focusing more specifically on electrochromism (V_2O_5) and thermochromism (VO_2) [2]. In addition, of the single layer characterization, the optimization of the architecture of the ECD multilayer device, also described as an optical battery, will be discussed in respect of the nature of the transparent conducting layer as well as of the electrolyte.

References

[1] I. Mjejri et al., Inorg. Chem., Low-Cost and Facile Synthesis of the Vanadium Oxides V_2O_3, VO_2, and V_2O_5 and Their Magnetic, Thermochromic and Electrochromic Properties, 56 (2017) 1734−1741

[2] I. Mjejri et al., From the Irreversible Transformation of VO_2 to V_2O_5 Electrochromic Films Inorg. Chem., in press 2022 DOI: 10.1021/acs.inorgchem.2c02722

[3] C. Périé et al., Colored electrolytes for electrochromic devices, Sol. En. Mat. Sol. Cell, 2022, 238, 111626

KEYNOTE SPEAKER

Pablo Ordejón
Director of the ICN2 - Institut Català de Nanociència i Nanotecnologia

Prof. Pablo Ordejón obtained his PhD (1992) at the Autonomous University of Madrid. He was worked at the University of Illinois (UAB), Universidad de Oviedo (Spain) and CSIC (Spain). In 2007 he moved to the Catalan Institute of Nanoscience and Nanotechnology (ICN2), of which he has been director since 2012. His work focuses on the development of methods for first-principles simulations of materials, and their application to problems in nanoscience. He has published more than 220 scientific articles, with more than 35,000 citations. He has been head of the Condensed Matter Physics area of the Spanish Evaluation Agency and of the Physics and Engineering Panel of the Spanish Supercomputing Network, and coordinator of the Physics area of the Gadea Foundation. He is Fellow of the American Physical Society and a member of the Academia Europaea, and received the Narcis Monturiol medal from the Government of Catalonia. He was co-founder of SIMUNE Atomistics SL, a spin-off company that provides materials simulation services to industrial clients.

Presentation ID: KN2 *Type of Presentation: Oral*

DFT and QM/MM simulations of electrified interfaces using Non-Equillibrium Green's Functions

P. Ordejon[1]*

[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus Bellaterra, Barcelona, 8193 Spain*

Understanding the interface between electrolytes and electrodes, specially when the latter are electrified, is an important but open problem. First principles atomistic simulations have so far been unable to describe with these systems, either due to the difficulty in treating the electrified interface, or because the number of atoms involved makes the computational cost prohibitive. We have developed methods that can tackle these problems, using a combination of DFT with Non-Equilibrium Green's functions to describe the effect of the potential applied to the electrodes. Further combining these quantum calculations with classical molecular dynamics using classical interaction potentials (so called QM/MM methods) allows us to scale up the simulation sizes and times to make these studies feasible. I will show some demonstration cases that show the potential of the approach in the study of aqueous solutions in contact with electrified metallic surfaces.

i3N THEMATIC LINES

TL1 – Sustainable Micro and Nanofabrication (FCT NOVA)

TL2 – Green and Clean Energy Systems (FCT NOVA)

TL3 – Nanomaterials Engineering and Functional Interfaces (Aveiro)

TL4 – Biomedical Devices and Systems (Aveiro)

Presentation ID: OTL1 *Type of Presentation: Oral*

Thematic line 1: Sustainable Micro and Nanofabrication

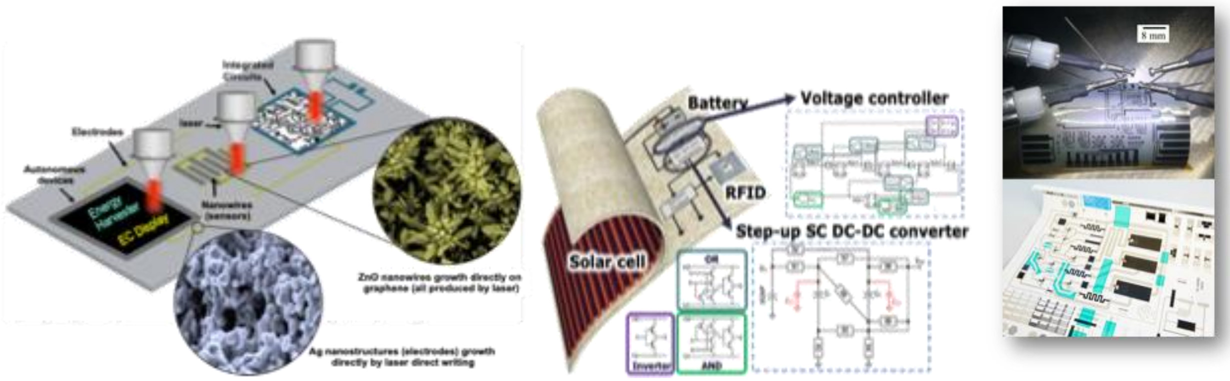
Rodrigo Martins
AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal;

The aim of this presentation is to show the road map related to the thematic area of micro and nanofabrication, where the main objectives foreseen are related to the: 1. Exploitation of sustainable materials for low cost electronic and sensing applications; 2. Adaptation of micro and nanofabrication using green technologies for sustainable electronics purposes, targeting mainly the so-called transparent and the paper electronics; 3. Explore multifunctionalities of metal oxides: integrated function vs integrated circuit; 4. Transition from conventional to flexible electronics.

These objectives are pursued by the different groups whose activities are focused on: modelling and simulation; nanoimprint methodologies; direct laser writing; plasma-assisted atomic layer deposition-based conformal coatings at low temperatures; system level design and integration; integrated control modules for rigid and mobile platforms, mostly away from silicon; power cube electronic systems; self-sustainable integrated circuits.

All these features will foster a wide range of important future focus areas of research and innovation in Portugal impacting in Europe, for a brighter future for all Europeans and mankind in general, for a sustainable and affordable electronics, for all.

The figure below aims to show what are the expected outcomes of this integrated activity and how this may impact over all of us.



a) b) c)

Fig. 1 – Examples of processing sustainable electronics devices and systems, away from silicon: a) direct laser writing; c) control systems on foils, full based on oxides; c) paper electronics examples

Presentation ID: OTL2 *Type of Presentation: Oral*

Thematic Line 2: Green & Clean Energy Systems

M. J. Mendes[1]*
[1] *AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal;*

Whether or not humanity is pushing the planet's life support systems over the edge depends largely on whether we can replace our dependence on fossil fuels with cleaner energy resources. In view of this goal, researchers at i3N have dedicated their work to push forward the boundaries of scientific knowledge and technical ingenuity in order to improve the conversion performance of several renewable energy technologies capable of harvesting power from widely-available sources (Solar with Photonic-enhanced Phovoltaics, Heat with Thermoelectrics, Vibration from Nano-generators, etc.). At the same time, we have been trailblazing means to enhance their market acceptance by pursuing cost-effective materials and fabrication processes, while also developing affordable energy storage plus integration solutions. Such R&D+I activities, undertaken at laboratory and pre-industrial level guided by advanced modelling and characterization, are presented here. Among a large number of scientific outputs with top quality, our expertise and commitment to a better Energy-efficient society has resulted in 11 Energy-focused projects which are running at i3N, adding to >10 M€ of competitive funds that are currently being managed only for within this thematic line. As an example, Figure 1 below depicts a targeted Solar Fuels implementation being pursued via some of these projects that are overviewed in this presentation.

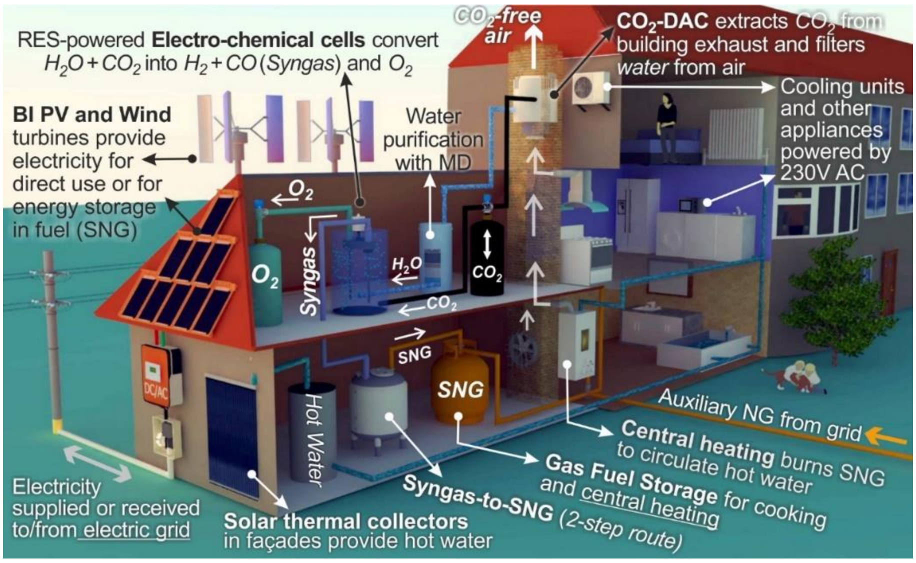


Fig. 1. Illustration of a projected implementation of a self-powered zero-emission building where the energy capture, conversion and storage equipment is installed in an annex (*left side*) that supplies energy to a larger building or condominium (*right side*). CO_2 flowing in the building exhaust is captured, to be converted to synthetic natural gas (SNG), all powered by renewable energy.

Presentation ID: OTL3 *Type of Presentation: Oral*

Thematic Line 3: Nanomaterials Engineering and Functional Interfaces

Luiz Pereira

1 FSCOSD/i3N, Department of Physics, Univesity of Aveiro Portugal

The ongoing work in nanomaterials engineering and functional interfaces is focused on developing and processing materials and nanoparticles for various applications including energy, optoelectronic, electronic, and bio applications. The activity areas are divided into several categories, namely processing and development of materials for energy, optoelectronic, and electronic applications, engineering of smart nanoparticles and 2D materials, laser processing and surface modification, and natural and bioinspired nanomaterials. The work has been carried out to functionalize interfaces to serve multiple applications.

The researchers have been studying the physical and chemical properties of the materials, as well as optimizing their synthesis parameters to achieve maximum performance in various applications such as solid-state light emitters, sensors, energy harvesting and storage media, and advanced functional nanomaterials and surfaces for health applications.

Additionally, efforts has been made on sustainable nanotechnologies for an innovative and industrially scalable methods. The research conducted has been extensive and includes different devices at interface layer such as solar cell, nanogenerators, transistor, sensors, among others.

An overview regarding the last achievements made on this fundamental research area, will be presented.

Presentation ID: OTL4 | *Type of Presentation: Oral*

Thematic Line 4

Author
Affiliation

i3N RESEARCH GROUPS

AFMMN – Advanced Functional Materials for Micro and Nanotechnologies (FCT NOVA)

PAMD – Physics of Advanced Materials and Devices (Aveiro)

SBMG – Soft and Biofunctional Materials Group (FCT NOVA)

TCP – Theoretical and Computational Physics Group (Aveiro)

SM – Structural Materials (FCT NOVA)

NO – Nanophotonics and Optoelectronics (Aveiro)

Presentation ID: OGR1 *Type of Presentation: Oral*

Advanced Functional Materials for Micro and Nanotechnologies (AFMMN) - FCT-NOVA

P. Barquinha[1]*
[1] *AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal*

During 2022 the Advanced Functional Materials for Micro and Nanotechnologies (AFMMN) Group pursued activity in four strategic lines of i3N: i) Sustainable Micro and Nanofrabrication; ii) Green and Clean Energy Systems; iii) Nanomaterials Engineering and Functional Interfaces; iv) Biomedical devices and systems, aligned with the Advanced Materials 2030 Initiative.

Key achievements were the demonstration of large-scale printing of zinc-tin oxide diodes, a smart textile display system with multifunctional fibre devices, a smart IoT enabled interactive self-powered security tag designed with functionalized paper, a flexible active crossbar array using amorphous oxide semiconductor technology toward artificial neural networks hardware, photonic-structured perovskite solar cells, water peel-off transfer of electronically enhanced, paper-based laser-induced graphene for wearable electronics, and carbon-yarn-based supercapacitors with in-situ regenerated cellulose hydrogel, also targeting wearable electronics.

All this work contributed to a sustainable, green and digital transition, being reflected in the accomplishment of all the dissemination KPIs for the period and in further competitive funds to the research centre. Highlights are provided below:

- >50 articles published in ISI journals, including Applied Physics Reviews (IF=19), ACS Nano, Nano Energy, Nature Communications (IF=18);
- >50 invited communications (including key-note and plenary) in prestigious international events (e.g., International Conference on Frontier Materials 2022, Zhuhai, China, or MRS Fall Meeting, Boston, USA)
- New competitive funding representing >14 M€ for FCT-NOVA, including 7 agendas in PRR program, an ERC PoC, 3 collaborative Horizon Europe projects, 1 collaborative Era-Net project and 5 national projects.
- Direct funding from international companies, worth >66 m€;
- 1 patent granted in USA, on radiation sensing oxide transistors, with commercialization routes being currently explored through an ERC PoC grant.

Presentation ID: OGR2 *Type of Presentation: Oral*

Physics of Advanced Materials and Devices (PAMD) – Aveiro

L. Cadillon Costa
PAMD-UA/i3N, University of Aveiro, Portugal

The core research in the PAMD group includes several investigation themes. It permits to consider different lines, in particular, wide band gap semiconductors and insulators, materials with enhanced electrical and magnetic properties, medical physics and instrumentation, carbon based materials and laser processing, and photovoltaic and optoelectronics materials and devices.

Optical characterization of wide band gap materials was conducted, in order to improve semiconductor capability devices and for sensing applications [1]. The development of high dielectric constant materials, such as ferrites, and also composites including barium titanate was done, allowing the use of electrical and magnetic storage energy. High-power microwave ovens to synthesize materials [2], and magnetic nanoparticles for hyperthermia was developed. The study of radiation detectors from gas ionization to organic and inorganic scintillation materials was done [3]. The technique use the last generation of silicon-based detectors, namely silicon photomultipliers, for applications in nuclear physics and medical instrumentation. Laser-processing of materials for structural and chemical modification, namely the production of laser induced graphene on eco-friendly materials for applications as embedded sensors/actuators and energy production/storage was performed [4]. Laser technology was further used for cleaning and surface engineering. The study of the optoelectronic properties of perovskites films, Si nanoparticles, NiO/Si heterojunctions, plasmonic Ag and Au nanostructures and the radiation hardness of solar cells was done. Fabrication of devices (OLEDs, LEDs, photovoltaics and chem/bio-sensors) based on organic and/or hybrid semiconductors was conducted [5].

The main achievements of the group in the last year will be reported.

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Presentation ID: OGR3 Type of Presentation: Oral

Soft and Biofinctional Materials Group (SBMG) – FCT NOVA

J.P. Borges[1*]
[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal

The Soft and Biofunctional Materials group (SBMG) is much involved in the study of soft materials, which are easily deformable by external stresses, magnetic, electric fields, or even by thermal fluctuations. The group has four main research areas: Liquid Crystals and Cellulose Liquid Crystalline Networks; Biomaterials; Rheology; NMR mand Rheo-NMR. The activities of the SBMG are alligned with the four thematic lines if i3N, with research involving both CENIMAT and AVEIRO hubs. The group studies focused cellulose nano objects, liquid crystalline cellulose and liquid crystal based soft systems, colloids, macromolecular systems, electrorheological fluids, elastomeric Janus particles, ionic liquids, poly(ionic liquids) and iongels, biomaterials, injectable hydrogels, cancer theranostics, electrical polarization and charging of polymers and ceramics applied to hard tissue regeneration, composite materials and devices. In this presentation a breif overview of most recent works of the group will be given.

Presentation ID: OGR4 *Type of Presentation: Oral*

Theoretical and Computational Physics Group (TCP) – Aveiro

A. L. Ferreira
TCP-UA/i3N, University of Aveiro, Portugal

Recent research done by members of the TCP group, in the research lines CNS – complex network systems, Computer modeling and artificial intelligence (CMAI), Ab-initio modeling in condensed matter AIMCM and Quantum transport (QT) is showcased.
The main research includes studies of weak percolation on multiplex networks with overlapping layers; epidemic models with application to COVID-19; localization of nonbacktracking centrality on dense subgraphs of sparse networks; Hidden phase transition in multiplex networks; model of synchronization applied to of non-identical swarmalators (CNS, [1]) C60 polymerization, modelling of elastic nanofilaments, applications of machine learning to food recipes (CMAI, [2]) studies of the degradation of solar cells, alloying-/pressure-engineering of semiconductors and radiation damage in solid state neutron detectors (AIMCM, [3]) and studies of extended 1D topological insulators; Hilbert space fragmentation and weak thermalization; noninteracting non-Hermitian n-partite tight-binding lattices (QT, [4]) .
The main achievements of the group in the last year will be reported.

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Presentation ID: OGR5 *Type of Presentation: Oral*

Structural Materials (SM) – FCT NOVA

J.P. Veiga[1]
[1] SM-CENIMAT/i3N, FCT-NOVA, Portugal

Highlights of the Structural Materials Group will be presented by the Group Responsible, showcasing the different areas of activity. The research covers functionally graded shape-memory alloys by solid state and additive manufacturing for multifunctional applications. Work is also being performed in the field of composite materials for problem-solving through computation and modelling for the analysis of tomographic imaging. In the area of additive manufacturing and fusion-based welding/processing, relevant achievements are being obtained, especially in the area of high entropy alloys. In the area of characterization of materials for historical and technological interpretation, work proceeds in the structural and corrosion study of Sn, Cu and bronze chalcolithic artefacts and in the study of ancient ceramic, porcelain, mortars and cement materials in historical monuments. Synchrotron radiation studies were widely used in the field of cultural heritage and metallurgical applications.

Presentation ID: OGR6 *Type of Presentation: Oral*

Nanophotonics and Optoelectronics (NO) – Aveiro

P. Antunes
NO-UA/i3N, University of Aveiro, Portugal

The recent research activities of the Nanophotonics and Optoelectroncis Group (NO) can be separated into two main areas, one more experimental aimed at the development and application of optical multipurpose sensor devices, and another one more theoretical and/or numerical, mainly applied in optical communications.

Among the various areas of activity, the following stand out: biomedical (biochemical, physiological and physical parameters, well-being and health, stress, body posture and cardiovascular biomarkers sensing); aquaculture/agriculture sector (contaminants in water, such as bacteria, nitrites and salts, density, temperature and turbidity, pH and salinity sensing); strain and temperature inside batteries, structural heath monitoring in buildings; development and application of innovative sensors based on microstructures and micro structured fibers with advanced geometries [1-4]; implementation of quantum protocols for key distribution [5] and simulation of nonlinear pulse propagation with applications in fiber communications, fiber devices, and lasers [6].

In 2022, the NO group published 51 articles in ISI journals and 4 book chapters, presented 17 communications in international conferences and 4 in national ones, organized 3 sessions in international conferences, had 1 finished PhD thesis and 10 Master dissertations concluded. New competitive funding, representing 772 k€ for i3N (with the PI from the NO group), was obtained from one FCT project and 1 PRR agenda project. Apart from that, several group members are participating in various other projects that started in 2022.

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Oral presentations by Ph.D. students

Presentation ID: OPS1 | Type of Presentation: Oral

Skin-interfaced, graphene-based bioelectronics for biomedical applications

T. Pinheiro[1,2]*, E. Fortunato[1], M. G. F. Sales [2], A. C. Marques[1], R. Martins[1]
[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal; [2] BioMark@UC, University of Coimbra, Portugal

Laser-induced graphene (LIG) has established itself as a very attractive material for electrode fabrication. The straightforward, high throughput graphitization of several precursor materials allows for the simultaneous synthesis and patterning of this 3D graphitic material with diverse electrode architectures, to target several biosensing applications, from biophysical to biochemical monitoring. Recently, paper has appeared as a viable alternative to conventional petroleum-based plastic polymer precursors, such as polyimide [1]. This is due to the possibility to photothermally convert aliphatic cellulose monomers into graphene lattices. Rational manipulation of chemical composition of substrates and modeling of CO_2 laser irradiation improves the graphitization potential of cellulose, to reach LIG film with 5 ohm.sq^{-1} sheet resistance and conductivities as high as 67 S.cm^{-1}.
In this presentation, we report the use of cellulose as a material in the toolbox of LIG precursors, aimed at the development of both disposable and wearable biosensing applications. Paper-based electrochemical sensors using this material are presented, aiming at disposable sensor development [2]. Glucose and pH electrochemical sensors were fabricated, showing the compatibility of the material with several sensing strategies. To translate patterned electrodes for wearable applications, a straightforward transfer method is presented, using a water-induced peel-off method, capable of efficiently separating unconverted cellulose and converted LIG phases, transfering LIG patterns onto flexible, conformable and elastomeric substrates, for example medical grade adhesives [3]. Using this method, electrochemical biosensors, strain sensors for biophysical monitoring and electrodes for electrophysiological signal monitoring are presented, aiming at the fabrication of robust point-of-care, disposable and wearable LIG-based analytical devices, aiming at more sustainable, accessible bioelectronic applications.

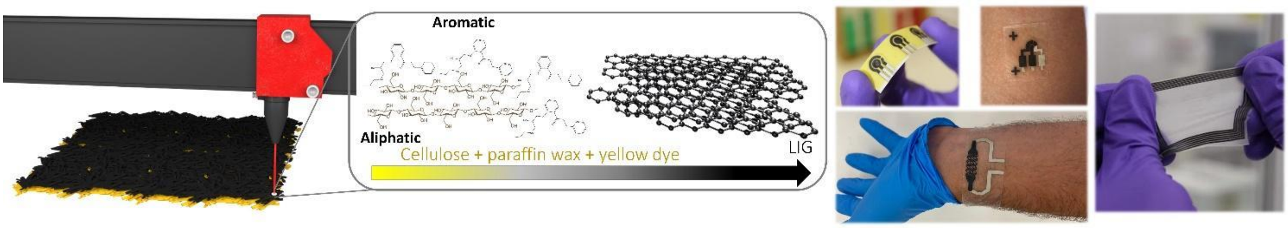

Fig. 1. Laser-induced graphene synthesis on paper and bioelectronic applications.

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Presentation ID: OPS2 Type of Presentation: Oral

Europium-Implanted AlN Nanowires: A Route for Red Nano-Emitters?

J. P. S. Cardoso[1]*, M. R. Correia[1], R. Vermeersch[2,3], D. Verheij[4,5], G. Jacopin[2], J. Pernot[2], T. Monteiro[1],S. Cardoso[4], K. Lorenz[4,5], B. Daudin[3], N. Ben Sedrine[1]

[1] DFis-i3N, Universidade de Aveiro, Portugal; [2] CNRS, Institut Néel, Université Grenoble Alpes, France; [3] IRIG-PHELIQS, NPSC, CEA, Université Grenoble Alpes, France; [4] INESC-MN, Portugal; [5] IPFN, IST, CTN, Portugal

Realize efficient red light-emitting diodes (LEDs) based on group III-nitrides (III-Ns) is essential for the monolithic integration of red-green-blue (RGB) emitters, enabling the development of efficient white LEDs and full-color displays at micro- and nano-scale. However, in contrast to the very efficient blue InGaN/GaN LEDs, the need for high In compositions causes the red LEDs to have low efficiencies (below 10% [1]). Polarization effects, growth constraints, and compositional inhomogeneities are some of the problems that affect the efficiency of red InGaN/GaN LEDs.

Europium (Eu)-doped III-Ns emerged as an alternative to conventional multi-quantum well LEDs. In this case, it is possible to take advantage of their intense and atomic-like intra-4f^6 transitions, particularly the one involving $^5D_0$ and $^7F_2$ multiplets (620–625 nm), for obtaining red LEDs with good color purity. This strategy was already proven successful in realizing red LEDs, with multi-layered *in-situ* Eu-doped GaN LEDs achieving efficiencies close to 10% [2].

Still, there is room to improve the performance of Eu-doped III-N LEDs by incorporating Eu ions in efficient lattice sites, exploring co-doping to improve luminescence sensitization, or adopting different host matrixes. In that sense, AlN has been proposed as a promising host for Eu-implanted species due to its wider band gap, which results in lower thermal quenching of the Eu^{3+}-related luminescence, and superior resistance to implantation damage. AlN also benefits from its ability to withstand higher annealing temperatures than GaN. This is important because ion implantation requires posterior annealing to recover the induced lattice damage and optically activate the Eu^{3+} ions. Furthermore, a recent study showed that the luminescent properties of Eu^{3+} ions in Eu-implanted AlGaN nanowires (NWs) are improved when using hosts with higher Al-contents [3].

In this presentation, red LEDs based on Eu-implanted AlN *p-n* junction nanowires (NWs) will be demonstrated [4]. The current challenges and limitations of this approach and some of the adopted tactics to tackle them will also be discussed.

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Presentation ID: OPS3 *Type of Presentation: Oral*

Acetic acid in artisanal ciders: Monitoring strategies

A. I. Freitas[1,2*], A. C. Vieira[1,2], D. Pereira[1,3], J. Bierlich[4], J. Kobelke[4], J. C. Marques[1,2], M. S. Ferreira[1,3]

[1] i3N, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; [2] Faculty of Exact Sciences and Engineering & ISOPlexis – CASTA, University of Madeira, Campus Universitário da Penteada, 9020-105 Funchal, Portugal; [3] Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; [4] Leibniz Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena, Germany

Organic acids are compounds naturally present in various fruits, vegetables, and grains or are formed during fermentative processes. In fermented beverages like cider, low concentrations of acetic acid contribute positively to the product's organoleptic characteristics; however, abnormally high concentrations of this acid indicate microbiological contamination [1]. Thus, acetic acid is often regarded as an important quality and safety marker, and legal limits for its concentration in ciders have been implemented. While cider producers commonly use steam distillation followed by titration to determine volatile acidity, expressed in acetic acid concentration, in analytical chemistry laboratories, acetic acid is usually determined by high-performance liquid chromatography with photodiode detection. The application of this technique to artisanal ciders produced on the island of Madeira between 2017 and 2021 by four different producers provided acetic acid concentrations between 0.28 and 2.49 g/L. These values vary greatly between producers and production years and are, in some cases, above the legal limits imposed by local authorities [2]. So to help ensure a higher quality standard and safety of this product, more frequent monitoring of acetic acid levels is required. As a potential alternative to these time-consuming and expensive analytical techniques, we have developed a balloon-shaped optical fiber sensor, based on cladding modal interference, for the simultaneous measurement of acetic acid concentration and temperature. The sensor presented a sensitivity of 9.3 pm/g/L, measured for acetic acid solutions in a concentration range of 0 to 630 g/L, with a resolution of 0.36 g/L. A maximum sensitivity of 28 pm/ºC was attained for temperature, measured in a 15 °C range at around room temperature.

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Presentation ID: OPS4 *Type of Presentation: Oral*

Magnetic-polymeric nanoparticles as a platform for brain drug delivery

C. I. P. Chaparro[1,2]*, M. C. Cavaco[2], M. A. R. B. Castanho[2], V. L. S. Neves[2], J. P. Borges[1], P. I. P. Soares[1]

[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] IMM-JLA, FMUL, Portugal

Poly(lactic-co-glycolic) acid (PLGA) nanoparticles enhance drug pharmacodynamics and bioavailability, and when loaded with magnetic nanoparticles (MNPs) they can act as contrast agents for magnetic resonance imaging (MRI) [1]. These characteristics make them attractive for brain imaging and therapy. However, the application of nanoparticles (NPs) for brain drug delivery is hindered by the presence of the blood-brain barrier (BBB). The BBB is a natural defense against circulating toxic and infection agents that also prevents most therapeutic compounds from reaching the brain. BBB peptide shuttle (BBBpS), are small peptides that engage adsorptive mediated transport (AMT) across the BBB and allow brain uptake [2]. In this work, we propose MNPs-loaded PLGA nanoparticles functionalized with a BBBpS, as a platform for brain drug delivery. We produced nanoparticles with a size range of 110-145 nm. In the functionalization step 30% of fluorescently labeled BBBpS was conjugated to NPs surface (BBBpS-NPs), resulting in size alteration. The size increasing in 30 nm but zeta potential does not change significantly due to the low net charge of the BBBpS, ranging from -33.2 ± 0.6 mV before functionalization, to -31.2 ± 1.2 mV after functionalization. To test activity of NPs we first investigated the interaction with human brain endothelial cells (BEC) that make up the BBB. NPs internalization in BEC was evaluated through flow cytometry and fluorescence microscopy. The results reveal that BBBpS promotes internalization, with an increase in BBBpS modified NP, in comparison with naked NP, at 24h. Also, time-course evaluation of NPs internalization reveals a plateau at 12 h, suggesting an equilibrium between endocytosis and exocytosis. We will further test these NPs in *in vitro* models of the BBB and *in vivo* brain uptake.

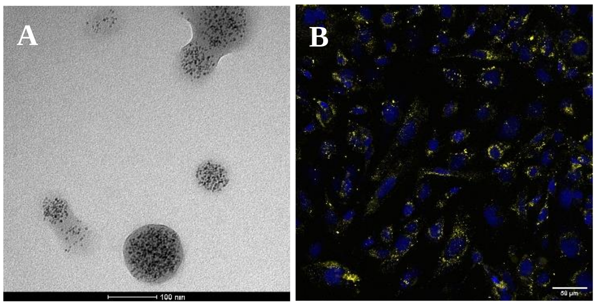

Fig. 1. (A) TEM image of MNPs-loaded PLGA nanoparticles. Scale bar = 100 nm. **(B)** confocal microscopy of NPs conjugated with BBBpS and internalized in BEC. Blue is Hoechst 33342 (nucleus) and in yellow are the BBBpS-NPs. Scale bar = 50 µm.

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Presentation ID: OPS5 Type of Presentation: Oral

Measures for causal network inference

F. Barroso[1]*, G. J. Baxter[1]
[1] TCP/i3N, University of Aveiro, Portugal

We propose a method to infer a causal network of a complex system from data, by evaluating a measure of association between events. Two events are said to be causally linked if the occurrence of one increases the probability of occurrence of the other. Thus, causal networks encode heterogeneous causal or influence relationships between objects in a complex system. Identifying the underlying causal network allow us to study the propagation of influences of events. These networks are called causal networks and they find applications in several areas, from production lines to telecommunication networks or medicine. However, the causal relationships in large complex systems are often not known, and relying on expert input for manual identification is heavily time-consuming. Thus, automatic ways of inferring causation are of prime importance.

HWe propose a normalized measure, similar to a certainty factor, that can be used to infer the likelihood of a causal relation. to validate this method, we computed weights from synthetic data. In order to generate the data, we created a random acyclic graph, with the condition that has a single sink node. Then we generated conditional random variables compatible with the graph and finally discrete values are generated according to those random variables. We can compare the most significant connections obtained with the ones in the original graph. A connection is deemed significant if its weight exceeds a threshold determined as the value immediately before the identified network ceases to be connected. This threshold can be identified quickly through binary search. The network can be further refined by identifying triangles and computing weights in the presence of a third variable. If for all combinations, the weights are close to zero, the connection can be deemed as created by a common cause and thus removed.

We find excellent agreement between the inferred network and the original synthetic network, as illustrated in Figure 1.

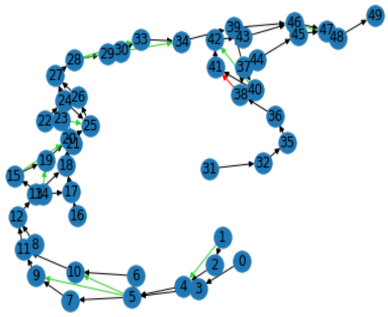

Fig. 1. Comparison of the inferred and original networks. In black the coincident edges, in red the missing edges, and in green the edges in excess.

Design and Production of Polymer-Based Composite Metamaterials via Fused Filament Fabrication: Methodology Overview

João O. Cardoso[1]*, João Paulo Borges[1], Alexandre Velhinho[1]

[1] *CENIMAT/i3N, Departamento de Ciência dos Materiais, Faculdade de Ciência e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal*

Throughout the development of this work there were constant alterations and revisions to the adopted methodologies. It is of interest to look back and share the process to better inform other researchers and supply them with broader research avenues. [1]

From the start, the goal was to create a methodology that was roboust enough to sytematically produce high-quality comparable results from diferent researched structures, while at the same time flexible enough that it could fit many different structures, materials and research paths (fabrication vs simulation). In addition to this, some degree of automation was possible to implement and the groundwork was done to perform structure optimization in the future.

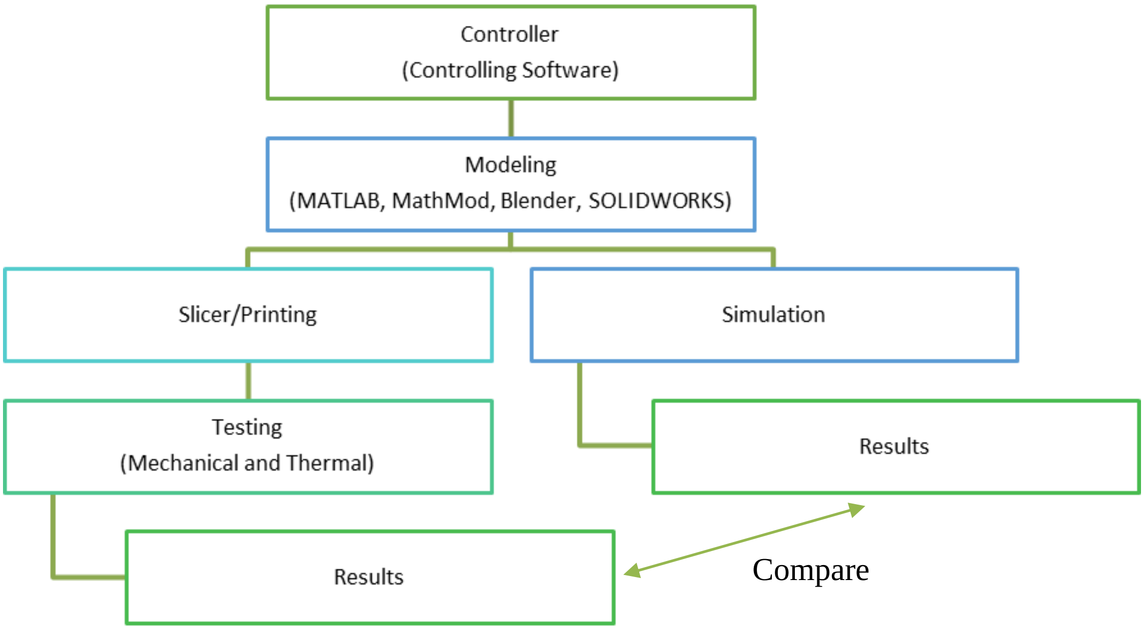

Figure 1 – Methodology Template Schematic

References

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Poster presentations

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Presentation ID: P1 Type of Presentation: Poster

In-memory computation: Amorphous oxide semiconductor memristors and transistors

Maria E. Pereira*, Jonas Deuermeier, Rodrigo Martins, Elvira Fortunato, Pedro Barquinha and Asal Kiazadeh**
[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal
*mel.pereira@campus.fct.unl.pt; **a.kiazadeh@fct.unl.pt

Neuromorphic computing is based on the development of device concepts which arise from biological neural systems. In this respect, innovative memristive devices have emerged as promising candidates to build extremely power efficient systems with high density for artificial intelligence applications, in-memory computing, and parallel processing technologies.

Memristors in crossbar arrays are essential core features of performing ultra-low-power artificial neural network (ANN) hardware. However, further development in certain criteria is required to be considered for an accurate ANN chip. Therefore, any proposed design should fulfill: 1. linear and symmetric synaptic weight update for multiply–accumulate (MAC) operation and 2. low cycle-to-cycle and device-to-device variability, as well as the 3. crosstalk issue for both inference and accurate training phases.

Here, we demonstrate on how to modulate the plasticity characteristic of a-IGZO memristors with low cycle-to-cycle variability. IGZO materials are promising candidates due to the great advantages in terms of low-cost manufacturing, stability, analog resistive switching, and compatibility with thin film transistors of the same material for full electronic support. We propose an a-IGZO-based memristor structure compatible with the monolithic integration of IGZO-TFTs. The transistor addition can solve the crosstalk effect. 1-transistor-1-memristor (1T1M) integration is presented by achieving an extremally high accuracy of 93.28 % for pattern recognition applications, unravelling the massive potential for the development of an efficient hardware for artificial neural networks applications [1].

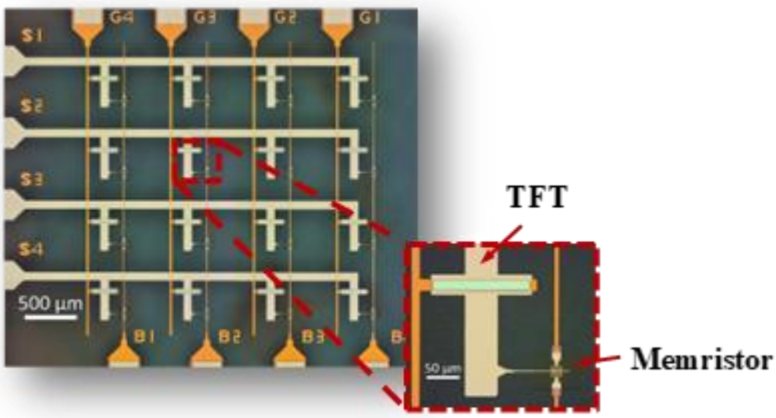

Fig. 1. 4×4 crossbar array of 1T-1R, IGZO memristor and TFTs

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Presentation ID: P2 *Type of Presentation: Poster*

Interface and surface engineering of CIGS films to improve cell performance

Sivabalan M Sivasankar[1*], António F da Cunha[1]

[1] PAMD, i3N-Aveiro, Department of Physics, University of Aveiro, Portugal, *sivabalanms@ua.pt

We are implementing processes to enable the production of high-quality CIGS films that are compact, have a high level of crystallinity, have large grains, and have minimal defects. To accomplish this, we are exploring remedies such as establishing optimum precursor order, introduction of thin metal oxide interlayers and alkaline impurity doping.

Contrary to what is widely accepted, we found, so far, that in a bi-layer precursor approach (i.e., Mo/CuGa/In or Mo/In/CuGa), the absorbers formed with CuGa in contact with Molybdenum resulted in very poorly performing cells. This was seen even though the CIGS layers were highly compact. On the other hand, absorbers formed with Indium in contact with Molybdenum resulted in poor adhesion between CIGS and Mo because of void formation at this interface and presented rough surfaces (Fig. 1). Nevertheless, the efficiencies of cells made from the latter absorbers were substantially better.

To try to improve the properties of the interface between Mo and CIGS, we introduced very thin (5-10 nm) layers of metal oxides such as TiO2 and Al2O3 on top of molybdenum using ALD. We found that with a 5 nm layer of TiO2 present a more uniform and compact absorber with better adhesion resulted (Fig. 2), while also allowing for a marginal improvement in cell efficiencies of 1%. However, we also noticed that the metal oxide used is also of significance, as although TiO2 showed advantageous effects, Al2O3 on the other hand resulted in non-functioning cells.

We also attempted alkali metal doping through KF evaporation on the CIGS surface to try to improve the absorber effectiveness but so far with limited success. We observed a nominal improvement of 1-2% on average between absorbers that had been treated with alkali metal and those that were not.

The depth elemental composition analysis performed using GDOES, is shown in (Fig. 3). It shows a Ga accumulation at the back of the absorber which leads to bandgap profile also shown. [1]

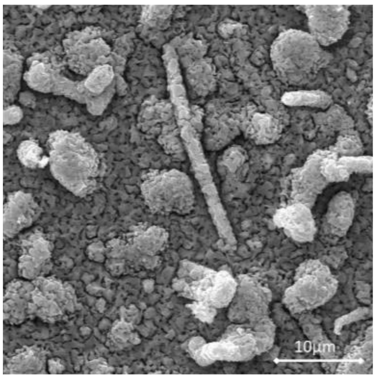

Figure 1: Surface Morphology with In at the bottom of the stack

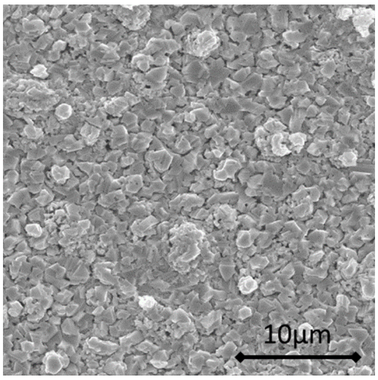

Figure 2: Morphology with addition of 5nm layer of TiO2

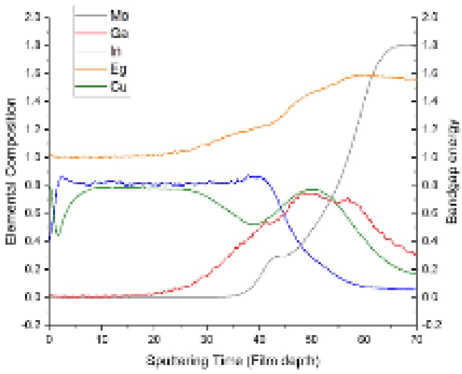

Figure 3: Energy Band profile calculated from elemental composition.

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Rheology as a tool for materials development

H. Carrêlo[1]*, C. Tipa[1], L.G. Baltazar[1], A.P.C. Almeida[1], P.L. Almeida[1,2], M.H. Godinho[1], J.P. Borges[1], C.R. Leal[1,2] e M.T. Cidade[1]

[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] Departamento de Física, ISEL, IPL, Portugal

Rheology appears as a powerful tool to provide the characterization of the mechanical properties under controlled conditions, allowing to explore and to develop new materials. The mechanical behavior under a simple shear flow can be characterized by the viscosity and normal stress differences, and when under oscillatory flow the elastic and the viscous modulus can be measured. Many other physical characteristics can be accessed and revealed by rheology, specially when combined with other measurements, as used in electrorheology, in rheo-optics or in rheo-NMR.
In this presentation will be displayed a diversity of rheological studies on different systems such as: biological and biocompatible material systems [1-5] and sustainable grout materials [6,7].

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Presentation ID: P4 *Type of Presentation: Poster*

Topological lattice models with complex geometries

A. M. Marques[1]*, E. Nicolau[2], J. Mögerle[3], G. Pelegrí[4], S. Flannigan[4], J. Mompart[2], V. Ahufinger[2], A. J. Daley[4], R. G. Dias[1]

[1] TCP, Department of Physics & i3N, University of Aveiro, 3810-193, Portugal; [2] Departament de Física, Universitat Autònoma de Barcelona, E-08193 Bellaterra, Spain; [3] Institute for Theoretical Physics. III and CIQST, University of Stuttgart, 70550 Stuttgart, Germany; [4] Department of Physics and SUPA, University of Strathclyde, Glasgow G4 0NG, United Kingdom;

**anselmomagalhaes@ua.pt*

We provide an overview of our most recent work, which covers different aspects of topological phenomena in lattice models. These range from investigating the behavior of ultracold bosons in staggered lattices of rings carrying orbital angular momentum, to the behavior of decorated square lattices under magnetic fields, thermalization properties of diamond necklace models, as well as to the properties of non-Hermitian tight-binding systems in one-dimensional topological insulators. Common features of these models include complex tunnelings and/or long-range hoppings [1], which give rise to novel topological properties such as many-body Aharonov-Bohm caging [2], cascading Hofstadter butterflies in higher-root models [3], as illustrated in Fig. 1, multiple domes in the distribution of entanglement entropies [4], and a generalized Lieb's theorem in non-Hermitian systems with unidirectional couplings [5]. These works provide detailed analyses of the underlying mathematical structures and physical mechanisms behind these phenomena, as well as experimental proposals for their observation in real systems, using a variety of artificial systems such as ultracold atoms, photonic lattices, and topolectrical circuits. The findings of this research may find application in the development of topological quantum technologies and quantum computation, and are of relevance for the understanding of new and exotic topological states of matter.

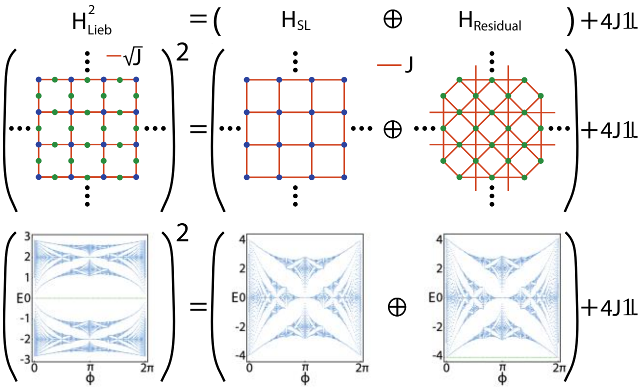

Fig. 1. Example of a square-root model, with its lattice structure and Hofstadter spectrum shown at the left-hand side, and the corresponding lattices and Hofstadter spectra obtained by squaring this model at the right-hand side (from [3]).

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Presentation ID: P5 Type of Presentation: Poster

Synthesis and characterisation of faceted Cu2O nanocrystals

Z. Cruz-Serrano[1]*, N. Bundaleski[2], E . Fortunato[1], R . Martins[1], J. Deuermeier[1**]
[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal; [2] CEFITEC, Department of Physics, School of Science and Technology, FCT-NOVA, Portugal

Efficient charge separation is a key element of a photocatalyst, aiming to provide electrons and/or holes to the reaction at the catalyst surface before they recombine inside a semiconductor. Built-in electric fields, which depend on crystallographic surface orientation, are the main driving force for charge separation. Synthesis and detailed characterisation of facetted nanoparticles is a first step towards resolving surface contributions of individual facets and their synergy in different photocatalytic processes e.g., water splitting or CO2 reduction. Recently, several simple procedures were proposed for synthesis of faceted Cu2O nanocrystals with well-controlled shapes and size. The band gap of this material is above 2 eV, making it a promissing absorber for creating the necessary high photovoltages for photocatalysis.
In this work we synthesized cubic and octahedral nanoparticles having approximate size of 200 nm, images of the samples obtained by scanning electron microscopy are presented in Fig. 1. Subsequently, heterojunctions were formed by depositing few nanometers of ZnO by atomic layer deposition (ALD). Identification of the nanoparticles' chemical phase was performed by means of X-ray photoelectron spectroscopy together with Raman Spectroscopy, before and after the deposition. In addition, the facet-dependent surface potential changes are discussed, completed by the work functions measured by ultraviolet photoelectron spectroscopy.

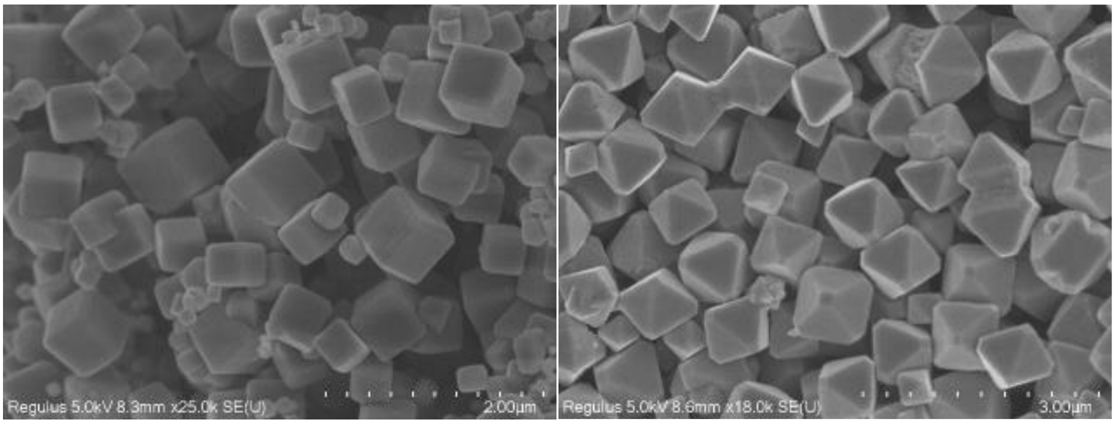

Fig. 1. SEM images of a) cubic and b) octahedral Cu_2O nanostructures

Presentation ID: P6 Type of Presentation: Poster

Development of environment-friendly epitaxial layers for energy-efficient solid-state refrigeration

E. Venkata Ramana[1]*, B. B. Chen[2], E. P. Houwman[2], M.A.Valente[1]
[1] PAMD, I3N, Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal
[2] MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

To reduce greenhouse gas emissions caused by the vapor-compression-based cooling technology currently in use, it is necessary to design low-noise and environmentally friendly refrigerants. Electric field-induced cooling can be viewed in this light as a promising and affordable on-chip cooling method that can be scaled down to small dimensions. Nanostructures with switchable polarization, near phase transitions, can exhibit large entropy changes that can be tuned by tailoring material properties.

Compared to bulk crystals, artificially engineered ferroelectric heterostructures such as epitaxial thin films, possess inherent advantages for easy integration in microelectronics with higher efficiency energy-recovery strategies. In the present work, we designed and investigated caloric effects in epitaxial oxide heterostructures of a promising polymorphic ferroelectric. High-quality $(Ba,Ca)(Ti,Zr)O_3$ (BCZT)–based thin films (15 – 375 u.c.) were been grown on SRO/STO substrates by the pulsed laser deposition. In-depth x-ray diffraction and dielectric measurements revealed a broad second-order-type phase transition around 440 K in 375 u.c thin films. A larger adiabatic temperature change (11.8 K) with an extremely broad temperature span over a wide working temperature range (350-440 K) resulted in enhanced relative cooling powers under the maximum electric field of 650 kV/cm. Experimental results, in comparison with bulk and thick films, are presented.

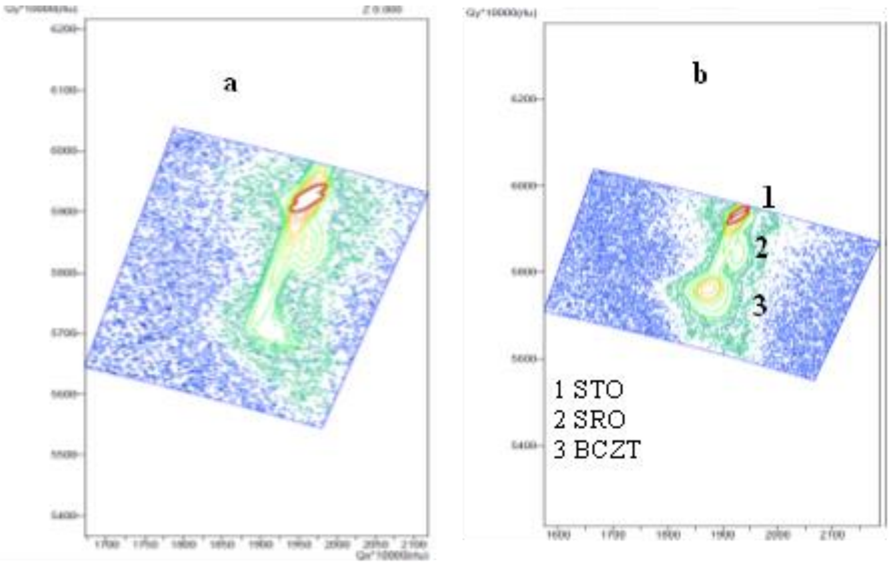

Fig. 1. {103} Reciprocal space map of (a) 15 u.c, (b) 375 u.c. BCZT/SRO/STO (100) thin film.

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Three millennia fine goldworkings: the Gold.PT project

E. Figueiredo[1]*, S. Serrano[1], R.J.C. Silva[1], A. Rodrigues[2]
[1] SM-CENIMAT/i3N, FCT-NOVA, Portugal; [2] VICARTE, FCT-NOVA, Portugal

Many of the decorations we find nowadays in gold and silver jewellery proceed from a long history of material experimentation and innovation. The archaeological jewellery collection present at the exhibition "Treasures of Portuguese Archaeology" in the National Archaeology Museum (MNA, Lisbon, PT) represents the largest asset in Portugal with Iron Age (second half of the first millennium BC) silver- and gold-workings. More than 200 artefacts are present, including necklaces, earrings and vessels, that by themselves incorporate various complex metalworking techniques, such as filigree, granulation, gilding, sheet-metal works, and diverse joining techniques. Gold.PT project (2022.02608.PTDC) aims to set-up a firm step on the creation of scientific and public comprehensible information on the Iron Age fine-gold working techniques, which were introduced and developed in the Portuguese territory more than 2 thousand years ago. Hence, 111 artefacts from MNA (earrings, necklaces, torcs, vases, among others; 34 silver-based) have been analysed for elemental composition by portable XRF and surfaces' recorded by multi-focus microscopy. Also, some artefacts have been studied in FCT-NOVA by SEM-EDS and micro-XRF for detailed information about gilding techniques and surface element depletion due to corrosion processes.
In this poster gold workings are shown which reveal the extremely fine techniques conceivable with the tools and knowledge of the people 3 millennia ago. Examples include the manufacturing of wires reaching diameters as small as 200 micrometers by the strip twisted technique (instead of the more modern drawn wire technique) and the production of silver gilded objects without the use of the (more modern) mercury amalgam technique.

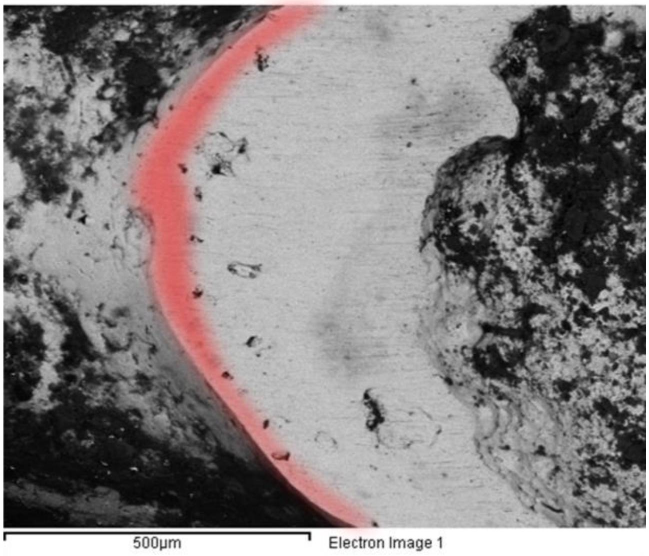

Fig. 1. At left a multifocus OM image detail of a 2 thousand years earring with gold wires of ~300µm diameter and granules ~1000 µm diameter. At right a SEM-EDS (BSE) image of a section of a gilded silver earring with a gold-rich layer ~40 µm thick (higlighted in red).

Presentation ID: P8 Type of Presentation: Poster

Optofluidic sensors: towards real-time characterization of liquid samples

J.M. Leça[1]*, Y. Magalhães[1], P. Antunes[1], V. Pereira[1,2], M.S. Ferreira[1]
[1] NO, i3N/Physics Department, University of Aveiro, Portugal; [2] ISOPlexis—Sustainable Agriculture and Food Technology Center, University of Madeira, Portugal, * jmleca@ua.pt

Optofluidics is a sensing technology area that combines elements of optics and photonics with microfluidic devices. Optofluidic sensing platforms are normally composed of microfluidic off-chip optical components as light sources and detectors and on-chip waveguides. The sensing mechanism is based on detecting changes in the optical properties of the liquid flowing media that can be used for its characterization in real time. Incorporating optical fiber sensors into optofluidic platforms can promote the development of new analytical tools to simplify traditional analytical methods, such as wet chemistry techniques, spectroscopy, spectrometry, and chromatography [1].
In this work, a 3D-printed optofluidic fiber sensor was developed combining a microfluidic system with an optical fiber Fabry-Perot interferometer for the real-time measure of refractive index in liquid samples. The microfluidic platform was designed and 3D printed with Acrylonitrile Butadiene Styrene polymer. The sample flow (≈ 3.7 μL/s) was perpendicular to the Fabry-Perot cavity. The interrogation system was constituted by a broadband light source and a low-cost optical power meter detector and glucose solutions were used to characterize the sensor. The optical power shift was correlated with the refractive index and a sensitivity of -86.6 dB/RIU was obtained. The sensor resolution was 5.2×10^{-4} RIU with a good stability. The feasibility of the optofluidic sensor was confirmed through real-time dynamic analyses of refractive index (Fig. 1). The easy production, linearity, stability, and sensitive instantaneous response make this sensor a suitable candidate for the purpose and can be further explored to study molecular diffusions and liquid microenvironments. Future functionalizations in the fiber tips of the interferometer can also be used to detect target analytes or a specific group of compounds [2].

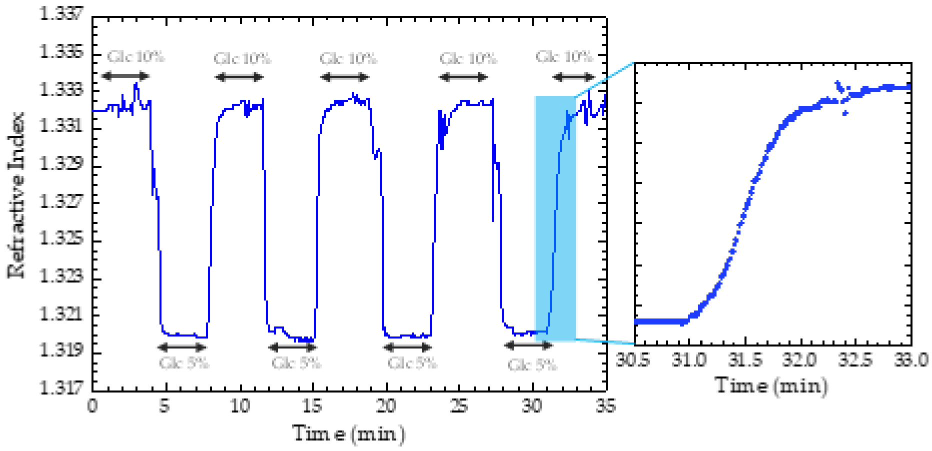

Fig. 1 Optofluidic fiber sensor real-time measurement of refractive index in transitions between samples of 5 wt.% and 10 wt.% of glucose (Glc).

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Presentation ID: P9 Type of Presentation: Poster

Atomic Force Microscopy: Probing the Interface Between Material Engineering and Biology

T. Calmeiro[1]*, H. Almeida[1], R. Martins[1], E. Fortunato[1]
[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal

Since its invention in 1986, atomic force microscopy (AFM) has cemented its place as a foundational technique in Nanotechnology. Its principle of operation, coupled with compatibility with a wide range of samples and different media of observation, makes it possible to observe and study phenomena at subnanometer resolution in native conditions or conditions similar to those in which a sample/device will be integrated and/or operated. These include liquid media or tissue culture media, unlike what other characterization techniques allow. This possibility is what made AFM a workhorse in research at the interface between Material Engineering and “soft” fields, such as Bioengineering, Molecular Biology, Biomedical Engineering, or Biophysics: characterization with minimal alteration.
In this poster, we selected a handful of case studies extracted from the characterization pipeline of both in-house and collaborative research, to highlight the added value generated by advanced AFM applications in different projects. The examples shown include the characterization of different phenomena, in diverse conditions, at different scales of magnitude, for various applications: from biomolecule characterization and interaction with other biomolecules (*e.g.,* DNA-protein interaction, protein networks) to biosensor proof-of-concept (*e.g.,* probe-target interaction and immunoassay surface activation), hydrogel characterization (mechanical and structural properties) or bioengineered organ tissues (mechanical properties).
AFM allows one to capitalize on the ever-growing need and interest in approaching materials and their characterization as close to their original properties and as close to their intended application as possible, assuring relevant characterization of materials and structures that would be negatively impacted by the requirements of other techniques.

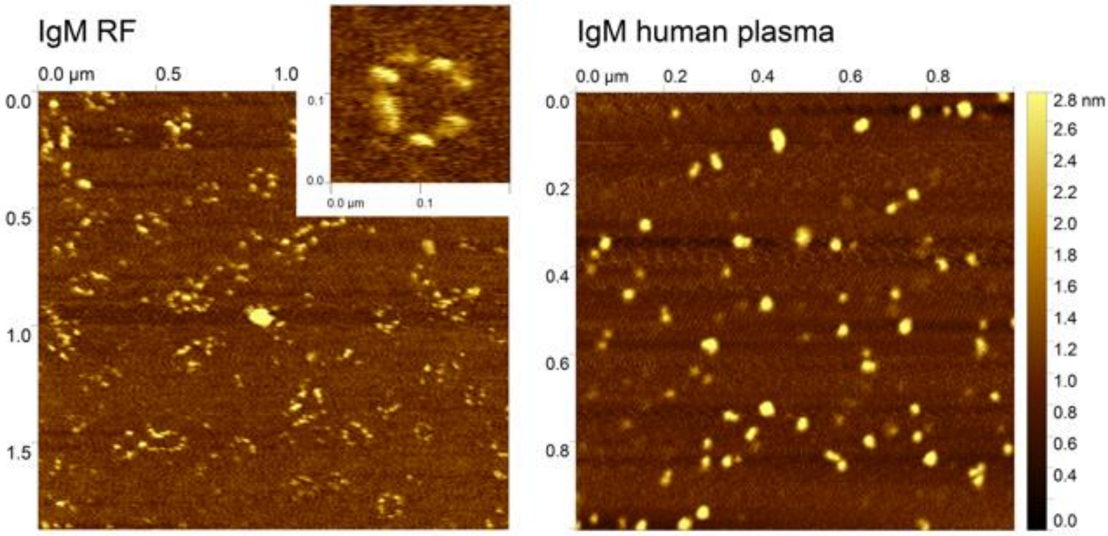

Fig. 1. Characterization of Au-nanoprobe-target complex for Rheumatoid Arthritis biosensor applications. Left: Positive result between IgM-Rheumatoid Factor (IgM RF) and Au-nanoprobes; Right: Negative result between IgM human plasma (control) and Au-nanoprobes.

Presentation ID: P10 Type of Presentation: Poster

Sustainable Paper-LIG Biosensors for Uric Acid Quantification in Urine

Bohdan Kulyk,[1,2] Sónia O. Pereira,[1] António J. S. Fernandes,[1] Elvira Fortunato,[2] Florinda M. Costa[1*] and Nuno F. Santos[1*]

[1] PAMD, i3N – Department of Physics, University of Aveiro, Campus Universitário de Santiago, Aveiro 3810-193, Portugal; [2] AFMMN, i3N/CENIMAT, Department of Materials Science and CEMOP/UNINOVA, NOVA School of Science and Technology, NOVA University Lisbon, Campus de Caparica, Caparica 2829-516, Portugal

Laser-induced graphene from paper (paper-LIG) was applied in non-enzymatic voltammetric electrochemical sensing of uric acid (UA) in human urine. Paper-LIG was formed by CO_2 laser modification of paper into an electrically-conductive porous 3D graphene arrangement.

Paper-LIG sensors can detect and quantify uric acid in phosphate buffer saline (PBS) within the 10 to 300 µM range at pH between 5.6 and 7.4. At pH 7.4, a linear response (R^2 = 0.999) from 10 to 250 µM was achieved, with a limit of detection of 3.97 µM and a sensitivity of 0.363 µA cm^{-2} µM^{-1}. The sensors denoted adequate selectivity in synthetic urine, dopamine and ascorbic acid (AA)-containing electrolytes. Determination of urinary UA content in human samples returned a concentration of c.a. 1.8-1.9 mM, within the range for healthy individuals. Recoveries of samples spiked with 50 and 100 µM UA were 100.6% and 95.4%, respectively, with satisfactory stability and reproducibility, even after one year storage at ambient conditions.

These cheap, lightweight, flexible, biodegradable and disposable paper-LIG biosensors for quantification of UA in human urine pave the way to widespread application in the detection of other important biomarkers at the point-of-care.

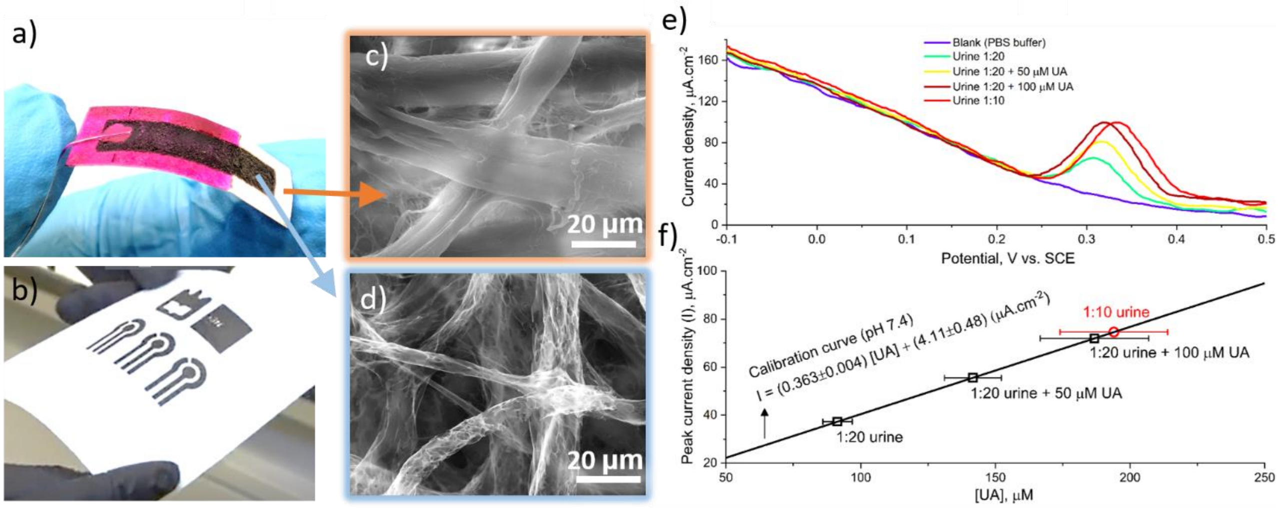

Fig. 1. Photographs of **(a)** Paper-LIG electrode and **(b)** Paper-LIG electrochemical cells. SEM micrographs of **(c)** paper and **(d)** LIG. **(e,f)** Electrochemical detection of UA in human urine.

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Presentation ID: P11 Type of Presentation: Poster

DREaMM: Engineering of dual-stimuli responsive nanofibrous magnetic membranes for synergistic cancer treatment

A. Gonçalves[1], R. Cabrita[1], J. Matos[1], I. Rodrigues[1], B. T. Simões[1], F. V. Almeida[1], S. N. Fernandes[1], M. Valente[2], T. Vieira[1], C. Henriques[1], J. P. Borges[1], P. I.P. Soares[1,*]

[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] PAMD, i3N/Physics Department, University of Aveiro, Portugal; *pi.soares@fct.unl.pt

The design, research, and development of new and improved smart structures and systems is currently a very hot topic in materials science and engineering. Nanotechnology has a huge potential for several applications, namely for the development of new biomaterials. The increased surface area and the optical, electronic, magnetic, and structural properties at nanometric scale are not available for bulk materials or individual molecules, making these materials unique.

The goal of project DREaMM is to engineer dual-stimuli responsive nanofibrous magnetic membranes based on a biocompatible thermoresponsive polymer and magnetic nanoparticles. In the present work, dual-stimuli responsive systems were developed by incorporating Fe_3O_4 magnetic nanoparticles (NPs) and poly(N-isopropylacrylamide) (PNIPAAm) microgels into electrospun polymeric fibers for application in cancer treatment. Fe_3O_4 NPs with an average diameter of 8 nm were synthesized by chemical precipitation technique and stabilized with dimercaptosuccinic acid (DMSA) or oleic acid (OA). PNIPAAm microgels were synthesized by surfactant-free emulsion polymerization. Poly(vinyl alcohol) (PVA) was used as a fiber template originating fibers with an average diameter of 179 ± 14 nm. Magnetic hyperthermia assays show that a higher concentration of NPs leads to a higher heating ability. The composite membrane with the most promising results is the one incorporated with DMSA-coated NPs, since it shows the highest temperature variation.

To assess the membranes biocompatibility and ability to promote cell proliferation, indirect and direct contact cell viability assays were performed, as well as cell adhesion assays. The present work demonstrates the potential of dual-stimuli composite membranes for magnetic hyperthermia and may in the future be used as an alternative cancer treatment particularly in anatomically reachable solid tumors.

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Presentation ID: P12 Type of Presentation: Poster

Innovative screening of critical issues in Aquaculture sector

M.S. Soares[1*], N.F. Santos[1], P.L. Almeida[2,3], C. Marques[1*]
[1] i3N & Physics Department, University of Aveiro, Portugal; [2] CENIMAT/i3N, FCT-NOVA University of Lisbon, Portugal; [3] ISEL, Polytechnic Institute of Lisbon, Portugal, *msimone.fsoares@ua.pt and carlos.marques@ua.pt

Along the entire Portuguese coast, is visible the presence of several estuaries, in which bivalve molluscs represent a significant proportion of the aquaculture sector. However, only small areas along the entire coast can be reached for the harvesting and commercialization of these aquatic organisms for direct human consumption due to the presence of *Escherichia coli* (*E. coli*). In addition, recirculating aquaculture systems (RAS) have been rising quickly in the last decade, representing a new way to farm fish by reusing the water in production [1]. Despite of the several advantages, fish biomass and water chemistry/quality interact and stress can be induced, as well as reduce food intake, reduce growth performance, and can also lead to mortality [2]. Furthermore, the presence of sub-micro/nano-plastics (sub-MP/NP) particles in the water tanks affects and causes the lowering of the metabolic and feeding rates as well as the body mass. Sub-MP/NP can also carry pathogenic bacteria [3], leading to fish-disease and epidemic infectious disease in farmed fish populations. In addition, it is critical to correlate all data from different sensing element and understand their interferences.

Currently, there is a huge gap in the global Aquaculture sector in terms of smart sensors for critical parameters, including cortisol (stress hormone), nitrites, bacteria, and sub-MP/NP (<1 μm) assessment. The objective is to create innovative biosensing, (e.g. in Fig. 1 for cortisol and *E. coli* detection, being also possible for nitrites detection), novel modalities and knowledge to overcome this gap, supporting European commercial innovation to preserve the fish well-being and food quality in line with the 2030 Agenda goals' objectives of European Union (EU) for sustainable aquaculture. It will contribute to accelerate the growth of aquaculture, allowing the achievement of the goals set by Food and Agriculture Organization (FAO) for 2030, to provide 62% of the fish consumed by man.

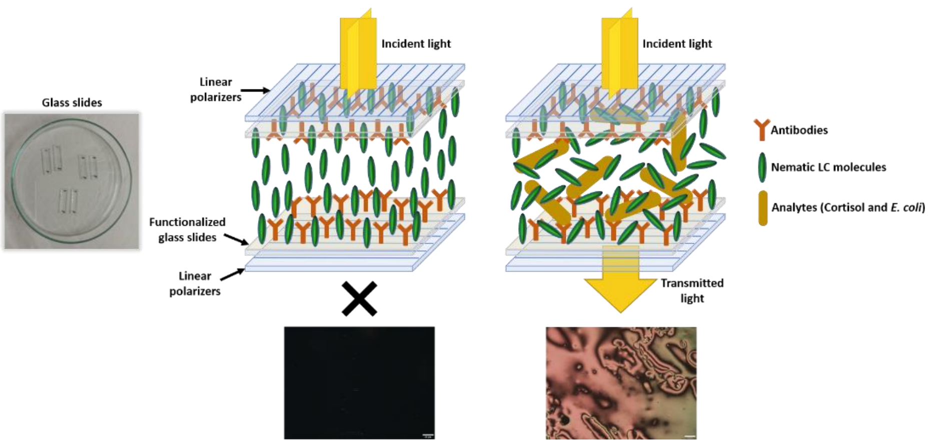

Fig. 1. Representation of portable liquid crystal-based polarization sensors for analyte detection.

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Presentation ID: P13 *Type of Presentation: Poster*

Wire and arc additive manufacturing of complex engineering alloys at the Structural Materials Group

Liu Lei, Jiajia Shen, Nithin Reddy, J. P. Oliveira [1]*
[1] *SM-CENIMAT/i3N, FCT-NOVA, Portugal, * jp.oliveira@fct.unl.pt*

Wire and arc additive manufacturing (WAAM) allows the creation of large metallic structural components, with the possibility to provide site-specific properties. Recent ongoing work at the structural materials group of CENIMAT/i3N has been focusing on WAAM of different engineering alloys, namely shape memory alloys of the Ni-Ti-X system [1] and high entropy alloys[2], but also for developing functionally graded components [3].

By combining process development, advanced microstructure and mechanical characterization coupled with thermodynamic predictive simulations it is possible to correlate how the processing conditions influence the microstructure and properties of the fabricated materials.

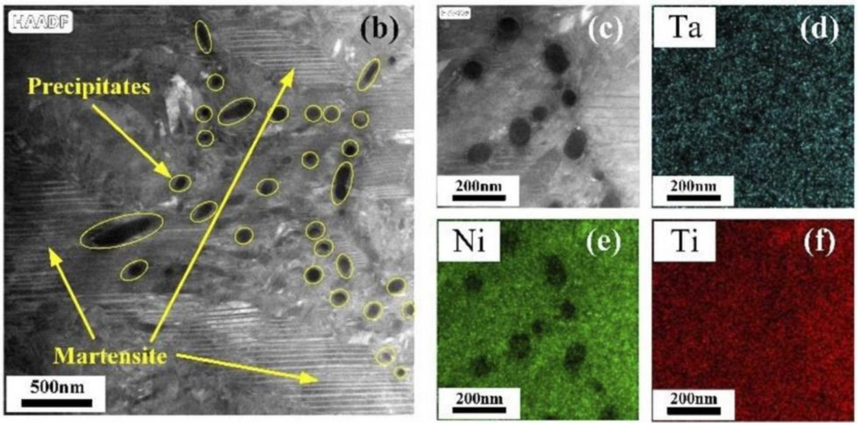

Fig. 1. TEM image of a NiTiTa high temperature shape memory alloy fabricated by WAAM.

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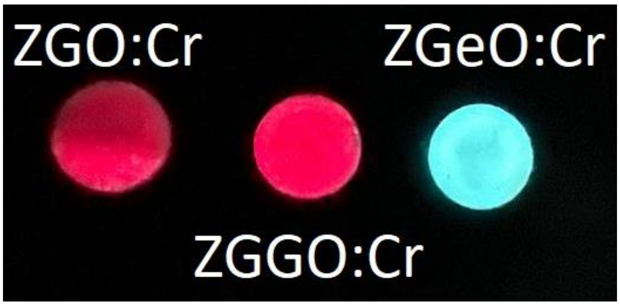
Presentation ID: P14 Type of Presentation: Poster

$Zn_{1+x}Ga_{2-2x}Ge_xO_4$: green and red persistent luminescence

Maria S. Batista[1]*, A. Violeta Girão[2], Florinda M. Costa[1], Ana Pimentel[3], Teresa Monteiro[1], Sónia O. Pereira[1]

[1] i3N, University of Aveiro, 3810-193 Aveiro, Portugal; [2] CICECO, Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal; [3] i3N/CENIMAT, NOVA School of Science and Technology, Campus de Caparica, 2829-516 Caparica, Portugal. * m.batista@ua.pt

Wide-bandgap oxides, such as $ZnGa_2O_4$ (ZGO), and Zn_2GeO_4 (ZGeO), have gathered much interest from the scientific community due to their significance for a variety of technological applications. Apart from this, the aforementioned materials present persistent luminescence characteristics, meaning that they can store energy from light irradiation, which upon cessation of the excitation is thermally released for a given time frame. Nowadays, they are of particular importance for anti-counterfeiting, optical information, night vision surveillance, photocatalysis, and optical probes in bioimaging, among other applications. One material that has spiked interest in the scientific community is the zinc gallogermnate (ZGGO, $Zn_{1+x}Ga_{2-2x}Ge_xO_4$), with bandgap energies around 5.0 eV at room temperature (RT). It is being widely studied over the past few years as a suitable host for doping with $3d^n$ transition metals ions, like Cr^{3+} ($3d^3$), to achieve long-lasting luminescence [1].
In this work, Cr-doped ZGGO pellets with different x values were produced via solid-state reaction in order to assess their structural, morphological, and optical properties. Being an alloy material of ZGO and ZGeO, its physical properties can be tunable depending on the concentration of Ge (x). For example, for x=0, the material presents a strong red/near-infrared (NIR) luminescence, whereas, for x=1, the luminescence consists of a green and red/NIR band [2,3] (Figure 1).



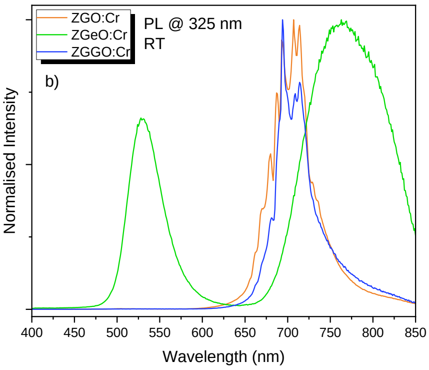


Fig. 1. a) Photograph of the pellets after cessation of excitation (254 nm); b) RT PL of the three samples.

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Presentation ID: P15 Type of Presentation: Poster

Study of Hydrothermally Synthesized ZnO Nanowires

M. Cortinhal[1]*, M. Morais[1], A. Rovisco[1], J. Martins[1], R. Martins[1], P. Barquinha[1]
[1]AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal. *m.cortinhal@campus.fct.unl.pt

One application of hydrothermally synthesized zinc oxide (ZnO) nanowire arrays is their use as semiconductors in vertical gate-all-around thin film transistors (GAATFTs) [1], which requires them to have a sizable length. In this study, the influence of hydrothermal synthesis parameters, including seed layer thickness and ultraviolet (UV)/ozone treatment time that this film undergoes, on the structural and morphological properties of ZnO nanowires was studied. The influence of synthesis temperature, time, and presence of surfactant were also evaluated. X-ray diffraction (XRD) was performed to evaluate the effects of an annealing treatment on the seed layer prior to the synthesis. This film was produced using Radio Frequency Sputtering technique. XRD and scanning electron microscopy were performed to determine the preferential growth direction and length of the nanowires. Regarding the seed layer, a 5-minute UV/ozone treatment and a 100 nm thickness produced the samples with the longest nanowires, with a length of 317 nm, which can be attributed to the synthesis procedure dynamics, since increasing any of these parameters proved to damage their vertical growth. For synthesis temperature and duration, 100 °C and 60 minutes produced the nanowires with the highest length. Using molybdenum as selective patterning, ZnO nanowires are then grown using the optimized synthesis, to be employed as a semiconductor in vertical GAATFTs, Fig.1.

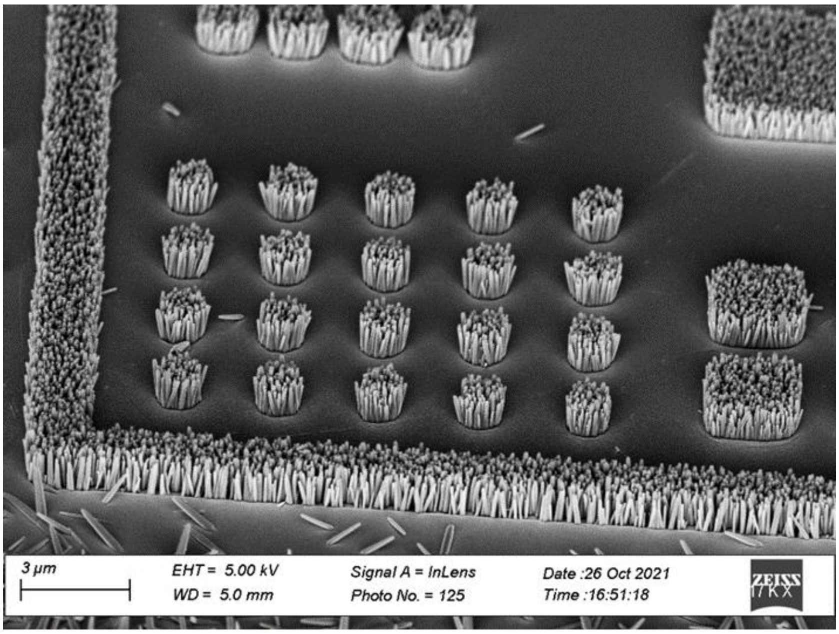

Fig. 1. Patterned ZnO nanowires.

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Dynamics of atomic and molecular hydrogen in silicon at finite temperatures from first-principles

D. Gomes[1]*, V. J. B. Torres[1], J. Coutinho[1]
[1] I3N, Department of Physics, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal. * dianafsg@ua.pt

The formation mechanism of hydrogen molecules in Si after quenching the material in contact with a hydrogen source from $T > 700$ °C to room temperature, is an intriguing problem that fascinated the community for decades. The puzzle is that at such temperatures the population of hydrogen is thought to consist of mutually repelling H^+ protons. Understanding this effect is particularly important in the context of the Light and elevated Temperature Induced Degradation (LeTID) of Si solar cells, which manifests after hydrogen being injected into the Si upon fast firing the cells [1]. We recently found that a boron-dihydride complex, formed upon capture of H_2 by boron, could be at the origin of LeTID [2]. Based on finite-temperature first-principles calculations, we found that the population of H^- cannot be neglected at high temperatures (Figure 1, left), allowing us to suggest that H_2 formation is Coulomb driven via $H^- + H^+ \rightarrow H_2$, and occurs during cooling after the firing step. This result also explains the mismatch between extrapolated diffusivities of atomic H measured at high temperatures (VWW data in Figure 1, middle) and low temperatures (GN data in Figure 1, right). While the calculated diffusivity of H^+ underestimates the high-T measurements nearly by a factor of 20 (line 1 in Figure 1, middle), the contribution of neutral and negatively charged species is found to significantly enhance the calculated effective diffusivity (line 2 in Figure 1, middle).

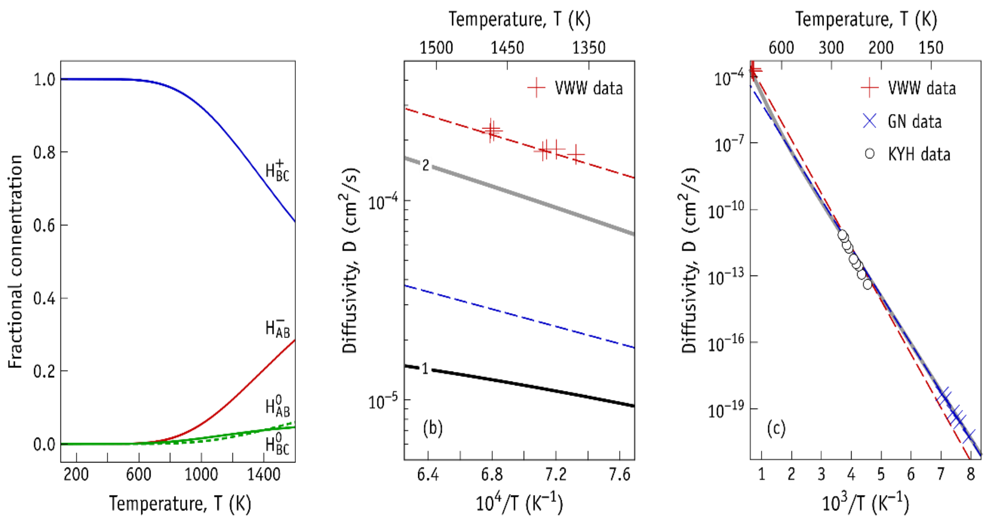

Fig. 1. Temperature dependence of the fractional population of several H atomic species in Si (left), high and low temperature diffusivity of atomic hydrogen in Si (middle and right, respectively).

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Presentation ID: P17 *Type of Presentation: Poster*

Bio-inspired sustainable optical security feature solutions from nanocellulose composites structural coloration

S.N. Fernandes[1]*, R. Chagas[1], A. Almeida[1,2,3], P.E.S. Silva[1], R.R. da Rosa[1]. P.I.S. Soares[1], P.L. Almeida[1,3], A. Baptista[1], J.P. Canejo[1], A.C. Trindade[1], J.P. Borges[1], L.F. Lopes[5], M. H. Godinho[1]

[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] LAQV/Requimte, DQ, FCT-NOVA, Portugal; [3] iBET, Portugal; [4] ISEL, IPL, Portugal; [5] IHMT, U. NOVA, Portugal

The NanoCell2SEC project aimed to create a platform of counterfeit-deterrence solutions derived from cellulose nanocrystals composites' structural colouration. These were fabricated from sustainable and cost-effective natural materials as cellulosic derivatives and inspired by the naturally observed reflection in insects. In the appropriate conditions, these systems self-assemble into liquid crystalline phases that can be fixed in matrices upon solvent evaporation or evolve with time, giving rise to structures with structural colouration. The iridescent structures (overt response) with selective circularly light reflection (covert response) allow an easy and effective security verification mechanism. Furthermore, active elements award increased security levels. The search for new insect biomimetic photonic structures contributed to a better understanding of their optical responses.

In this poster, an overview of the main achievements obtained in this project is done, which will include observation of insects [1], random laser systems [2], photonic composite systems with cellulosic derivatives [3], and time-dependent dynamic photonic systems [4], to state a few. In addition, outreach dissemination was a significant segment of this project, culminating in a scientific exhibition (Figure 1), showed at a national museum, where the curators and organisers portrayed in layman's language the main concepts behind this project.

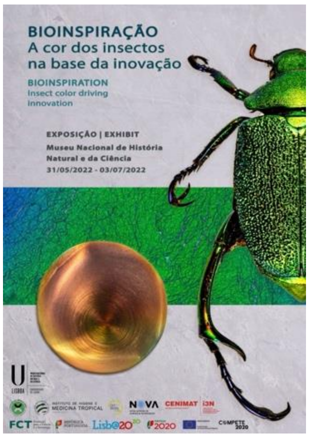

Fig. 1. Flyer of the exhibition with the title Bioinspiration: Insect color driving inovation presented at the *Museu Nacional de História Natural e da Ciência*, *Universidade de Lisboa* from 31/05-2/07/2022, under the framework of the project NanoCell2SEC (PTDC/CTM-REF/30529/2017).

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PET scanners based on an innovative acquisition method

F. M. Ribeiro[1]*, A. C. M. Magalhães[1], A. L. M. Silva[1], A. X. Pinto[1], B. Cruzeiro[1], I. F. Castro[2], J. Borges[1], P. M. C. C. Encarnação[1], P. M. M. Correia[1], R. G. Oliveira[1], J. F. C. A. Veloso[1]

[1] PAMD/i3N, Physics Department, University of Aveiro, Portugal; [2] RI-TE Lda., University of Aveiro Incubator, Portugal; *fabiana.ribeiro@ua.pt

Positron Emission Tomography (PET) allows to quantify the 3D distribution of a retained positron-emitting compound as a function of time. This non-invasive nuclear imaging technique studies and quantifies the functionality of different tissues in normal and diseased conditions, identifying cell behaviour alterations in the early stages of the disease.

The easyPET technology [1] (WO2016147130 A1/PCT/IB2016/051487) is an innovative PET imaging acquisition method based on a U-shaped board with two axes of motion and two modules of detectors always face-to-face, therefore, conducting to a significant reduction in the number of components compared to conventional scanners. Its non-conventional geometry allows the scanning of billions of lines of response in few minutes with less scatter and parallax error, compared with other scanner architectures.

The easyPET scanners are the lightest and most compact ones, saving space, simplifying infrastructure requirements, and reducing consequently costs. Therefore, these benchtop systems contribute to inclusive and equitable quality education and investigation while promoting learning and researching opportunities for all. The first easyPET system produced 2D imagens and was built for educational purposes, Fig.1 (A). Then, its complexity increased (Fig. 1 (B)) to the easyPET.3D, which can acquire the 3D distribution of the positrons, and to the easyPET.CT by adding the morphologic imaging capabilities to the scanners. Both are used for training health professionals and entry-level preclinical research. Moreover, those systems were adapted for applications such as zebrafish imaging and proton beam range verification, the fishPET and the HadronPET, respectively. The continuous development of the technology expanded the easyPET family to the iPET illustrated in Fig. 1 (C), suitable for advanced-level preclinical research, and to the BRAIN.PET, schematically shown in Fig. 1 (D), with clinical application in brain PET imaging. All scanners have the possibility to adjust the acquisition parameters, in particular the field-of-view diameter and the acquisition speed, according to the user's needs. PET images are reconstructed using a customized fast GPU-based iterative algorithm.

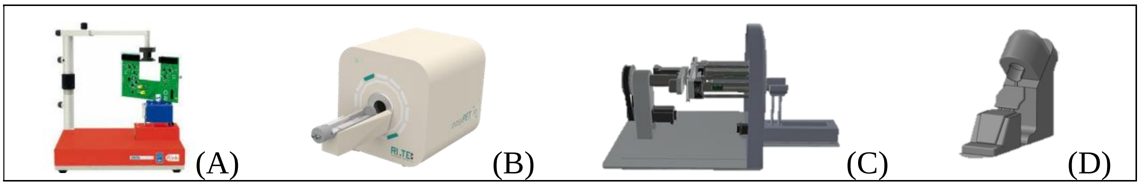

Fig. 1. easyPET family: (A) easyPET educational; (B) easyPET.3D, easyPET.CT, fishPET and HadronPET; (C) iPET; (D) BRAIN.PET.

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Presentation ID: P19 Type of Presentation: Poster

Flexographic printed thermochromic stickers with visible color transition for smart sensing applications

M. Morais[1,*], J. Figueira[1], E. Carlos[1], M. C. Corvo[2], C. Marques[1], A. Gonçalves[1], R. Martins[1] and J. V. Pinto[1]

[1] MEON-CENIMAT/i3N, FCT-NOVA, Portugal, [2] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal;
*md.morais@campus.fct.unl.pt

Smart packaging and temperature control are two areas where the search and development of new high-performance thermochromic materials are a key focus. Thermochromic materials have the ability to change their optical properties, either reversibly or irreversibly, depending on the reaction behind their thermochromism. In this work, a thermochromic material based on complexes of 1-butyl-3-methylimidazolium chloride and tetrachloronickelate ($[BMIm]_2[NiCl_4]$) was produced during a coordination reaction between BmimCl and nickel chloride hexahydrate according to a previously established procedure [1]. These thermochromic complexes present promising features, such as high color contrast and low-temperature transition (between 30 and 40 ºC). In this work, they were, for the first time, incorporated in printable inks based on cellulose derivatives that can be printed on flexible substrates, such as paper and commercial tags. The produced flexo-printed thermochromic stickers, whose fabrication process is presented in Fig. 1, are affordable and conformable platforms that can be used in various applications. The influence of the thermochromic material's concentration and the nature of the cellulose derivative present in the ink on the response time and color contrast were studied. This work opens the door to the development of easy-to-produce stickers with a fast response and high color contrast that enable a rapid and simple inference of the instantaneous temperature of a specific surface.

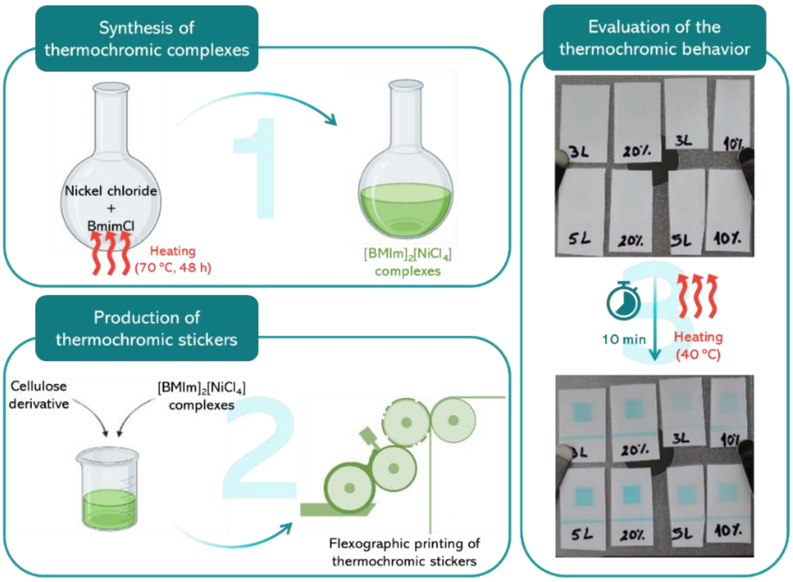

Fig. 1. Stages for the production of thermochromic stickers by flexographic printing.

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Optical biosensing platform for point-of-care monitoring of heart failure patients

M. Vidal[1]*, A. S. Assunção[1], L. I. Segerink[2], A. Morrin[3], S. O. Pereira[1], C. Leitão[1]
[1] i3N, Department of Physics, University of Aveiro, Portugal; [2] BIOS Lab on a Chip group, Technical Medical Centre, MESA+ Institute for Nanotechnology, University of Twente, the Netherlands; [3] National Centre for Sensor Research, Dublin City University, Ireland;
**miguelvidal@ua.pt*

Heart failure (HF) and sudden cardiac death (SCD) are widely concerning public health problems, whose prevalence is rising due to population growth and ageing. Regular HF assessment is essential to identify disease progression and is generally performed by measuring biomarkers, such as N-terminal pro-B-type natriuretic peptide (NT-proBNP) and electrolytes, along with physiological signals including heart rate, blood pressure and arterial stiffness [1], [2]. Electrolyte measurement is important as imbalances like depletions of Mg^{2+} and K^{+} can trigger ventricular arrhythmias, being strong predictors of SCD [1]. Currently, biomarker analysis is mostly done resorting to laboratory-based methods, which are highly sensitive although bulky and time-consuming, hindering their application at point-of-care (POC) [3]. Thus, optical fiber biosensors have been explored as an alternative since they are small, electrically safe and fast [4]. Moreover, on-skin devices are popular for POC applications and can involve colorimetric biosensing, as well as biosignals' measurement by photoplethysmography (PPG), enabling rapid, continuous and non-invasive monitoring [5].
This research envisages the development of a POC optical biosensing platform (Fig. 1) for risk management of HF and SCD. This portable platform consists of three complementary devices, namely, gold-coated unclad optical fiber tip (Au-tip) for NT-proBNP detection in saliva, microfluidic biosensor for colorimetric measurement of sweat electrolytes (Mg^{2+} and K^{+}) and epidermal optoelectronic PPG sensor for biosignals' monitoring acquired from the carotid and femoral arteries.

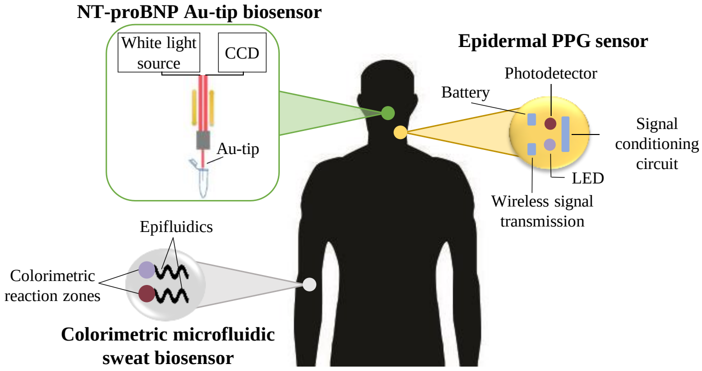

Fig. 1. Schematic illustration of the biosensing platform for biomarker measurement and biosignals' monitoring. CCD, charge coupled device; PPG, photoplethysmography; LED, light-emitting diode.

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Presentation ID: P21 Type of Presentation: Poster

Welding of high entropy alloys: thermodynamic modelling, microstructure and mechanical characterization

Nithin Reddy, Jiajia Shen, J. P. Oliveira [1]*
[1] SM-CENIMAT/i3N, FCT-NOVA, Portugal, * jp.oliveira@fct.unl.pt

Weldability studies on high entropy alloys are still relatively scarce, delaying the deployment of these novel materials into real-life applications. Thus, there is an urgent need for in-depth studies of the weldability of these novel advanced engineering alloys. The Structural Materials group of CENIMAT/i3N is currently leading an effort to establish processing/microstructure/properties in welded high entropy alloys from different systems [1–4].
By combining different welding processes, namely laser welding, gas metal and gas tungsten arc welding, alongside with thermodynamic modelling, advanced microstructure characterization encompassing synchrotron X-ray diffraction and electron microscopy, as well as mechanical testing, exciting advances in this field have been observed recently opening the door for the widespread use of the materials and processes in different applications.

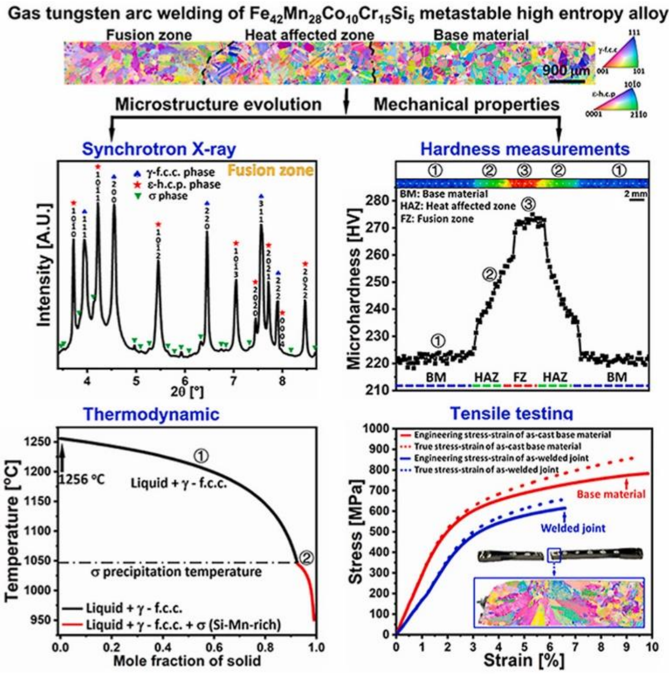

Fig. 1. Different approach to probe processing/microstructure/properties in welded high entropy alloys.

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Presentation ID: P22 *Type of Presentation: Poster*

Laser technology for different applications in industry

N.M Ferreira, R.M. Santos, A.J. Fernandes, A.F. Carvalho, F.M. Costa
PAMD - Physics Department & i3N, University of Aveiro, Portugal

In the last years, laser technology had great developments, becoming an easy handling processing technique with decreased environmental impact and maintenance requirements. Particularly, current industrial-grade lasers show high-performance in the local modification of the surface-properties of materials. In our group, we have been collaborating with different industries aiming at modernizing their processes through the application of laser technologies.
One application that takes advantage of this process is the fast and localized laser-cleaning which is most typically applied in rust removal, but that can also be applied to other challenges, namely mould cleaning [1]. Through the ablation process, the laser energy is used to remove the residues that are on the mould surface without damaging the mould composition and structure. Unlike other techniques, such as chemical etching, where the solutions used for cleaning become contaminated and create residue management issues, the laser-cleaning technique is an eco-friendly and efficient approach. Complementarily to this cleaning process, lasers can be also applied for coating removal in the mould industry [1].
The ceramic and glass industries are other examples where laser-processing is explored to reduce energy costs. By selectively processing areas of the parts, some steps that traditionally require the full parts to undertake a treatment in the oven can be replaced by the localized heating through a laser source [2,3]. These energy savings are particularly relevant today considering that most of these processes are conducted in gas-fuelled furnaces, not only substantial CO_2 emitters, but also highly vulnerable to disturbances in this fuel supply-chains.

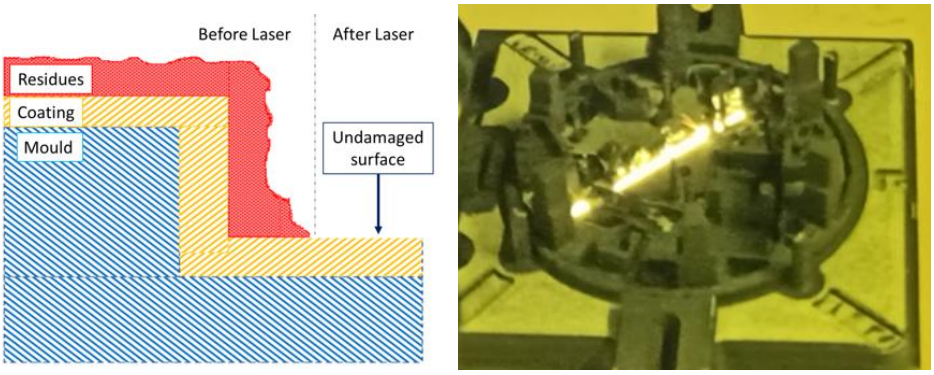

Fig. 1. Laser-cleaning a mould with residues. **Left** – schematic illustration of the process. **Right** – real-time photograph of the cleaning process over a complex shape.

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Presentation ID: P23 Type of Presentation: Poster

NMR as a tool for materials development

M. Corvo[1]*, P. Almeida[1,2], R. Barrulas[1], T. Paiva[1], M. Godinho[1], J. Borges[1]
[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] Physics Dep., ISEL, Portugal;
*marta.corvo@fct.unl.pt

Nuclear Magnetic Resonance spectroscopy (NMR) has become an essential analytical tool to solve a wide variety of problems in the field of chemistry, biology, and physics. In SBMG, NMR allows us to study the structure and dynamics of both small molecules and macromolecules, here, we highlight the use of solid-state (ss)NMR to study polymers and composites, magnetic resonance imaging (MRI) to develop contrast agents and study the morphology of complex systems, Rheo-NMR to study fluid dynamics under shear, and diffusion studies to study transport properties in ionic liquids and ion gels.
Relying on NMR to pave the way toward the development of new materials for CO_2 capture (CC) and conversion, project GREENPILs4CO_2 has taken full advantage of NMR techniques. CC has become an urgent matter in response to global climate change, thus, reducing greenhouse gas emissions requires the development of new materials and technologies. Commercial available CC technologies usually require high energy consumption or suffer from a decreased performance in the presence of impurities.
The main goal of GREENPILs4CO_2 was the development of materials for CC near atmospheric pressure, and upcycle CO_2, catalyzing the respective conversion. Initially, the affinity of ionic liquids (ILs) and poly(ionic liquids) (PILs) for CO_2 was studied using high-pressure NMR. The underlying molecular interactions were disclosed using NOE, relaxation, and diffusion NMR experiments, allowing the identification of the most promising candidates. These materials were incorporated in two main product lines - chitosan/IL/PIL composites in solvent mixtures for CO_2 capture at atmospheric pressure, and porous chitosan/PIL aerogels for CO_2 capture and conversion which were tuned using ssNMR. Finally, CO_2 was successfully converted to added-value compounds using PILs-derived aerogels, cryogels, and carbons.[1-3]

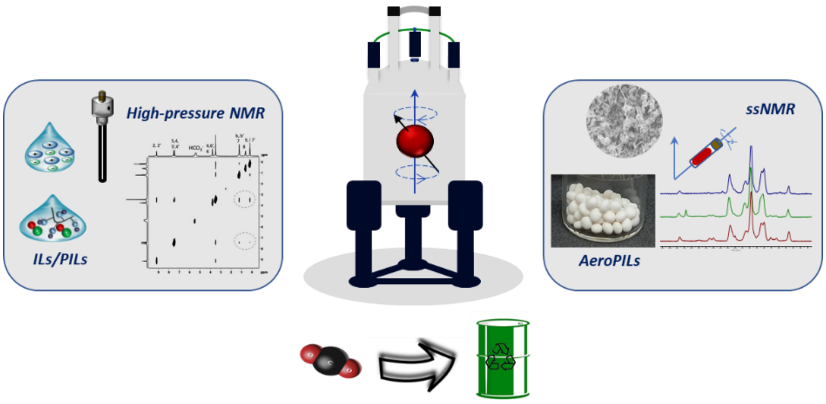

Fig. 1. General approach of GREENPILs4CO_2 project.

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Quantum Nanostructured Dots-in-Host Perovskite Solar Cells

M. Alexandre, H. Águas, E. Fortunato, R. Martins, M. J. Mendes
AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal

The outstanding physical properties of dots-in-host (QD@Host) hetero semiconductors demand detailed methods to fundamentally understand the best routes to optimize their potentialities for different applications. In particular, the intermediate band solar cell (IBSC) application, which is closely followed throughout this work.[1] A complete 4-band k.p-based method was developed for rocksalt quantum dots (QDs) that describes the complete optical properties of arbitrary QD@Host systems, trailblazing the way for the full optoelectronic analysis of quantum-structured solar cells. The 4-band model is built atop a 1-band model,[2] that can then expanded to a 4-band model that considers interband interactions, and thus the permits the calculation of the absorption coefficient. Here, the full model was firstly validated against well-established literature results. The electron transition rate was then determined and its dependency on the main compute parameters analyzed. This was followed by a multi-parameter optimization, considering intermediate band solar cells as a promising application, where the best QD configuration was determined (Figure 1a)), together with the corresponding QD@Host absorption spectrum (Figure 1b)), in view of attaining the theoretical maximum efficiency (50%) of this photovoltaic technology. The results show the creation of pronounced sub-bandgap absorption due to the electronic transitions from/to the quantum-confined states, which enables a much broader exploitation of the sunlight spectrum.

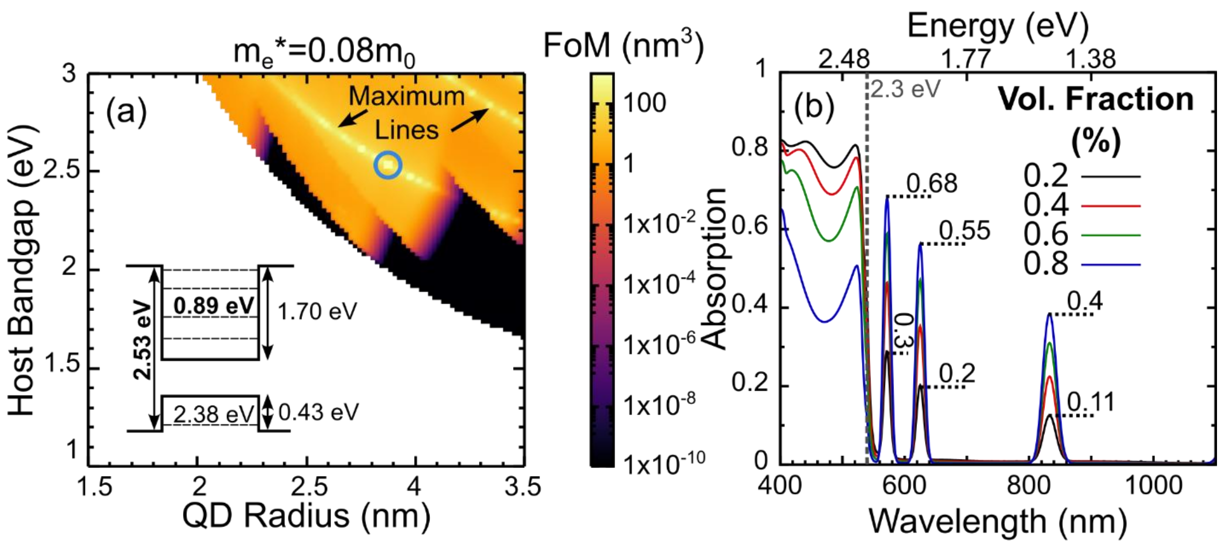

Fig. 1. a) Optimization profile for QD system with $0.08m_0$ effective mass; b) Scattering Matrix Method-determined single layer absorption for the best QD system optimized in a).

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Tailoring plasmon-enhanced light-harvesting in perovskite solar cells by using gold nanorods

Diogo F. Carvalho[1,2,3]*, Jennifer P. Teixeira[3], Manuel A. Martins[4], Pedro M. P. Salomé[2,3], Paulo A. Fernandes[1,3,5], M. Rosário P. Correia[1,2]

[1] i3N, University of Aveiro, Portugal; [2] Department of Physics, University of Aveiro, Portugal; [3] INL – International Iberian Nanotechnology Laboratory, Portugal; [4] I3S – Instituto de Investigação e Inovação em Saúde, University of Porto, Portugal; [5] CIETI, Department of Physics, ISEP – Porto School of Engineering, Portugal. *diogocarvalho@ua.pt

In recent years, several approaches have been developed to improve the performance of perovskite solar cells (PSCs). The photon capture ability is impaired at IR frequencies, because of the large decrease in the absorption coefficient for photons with energies lower than the bandgap of the commonly used perovskite absorbing layers (typically, 1.5-1.6 eV). Additionally, using a minimum thickness of the perovskite layer is of utmost importance to reduce the lead content and the related toxicological issues. As such, there is a demand for an optimization of the optical design of PSCs.

The incorporation of metallic nanoparticles (NPs) in the architecture of solar cells has been one of the strategies that, in theory, has shown the highest potential in increasing the performance of solar cells, and, more particularly, in PSCs [1]. The absorption enhancement offered by the NPs, mainly related to the near-field enhancement close to the NPs surface at the plasmonic resonance, could deploy the potential to use PSCs with ultra-thin perovskite layers. The plasmonic optical properties of NPs can be fine-tuned, and varying their shape is one of the most suitable approaches to do it. A few theoretical works have optimized the perovskite absorption for different NP sizes and concentrations [2,3]. Still, the optimization was done only for spherical NPs, and not always in realistic architectures (multi-layered structures).

This work numerically predicts the perovskite ($MAPbI_3$) absorption and near optical field distribution in realistic n-i-p PSCs embedding gold nanorods, the most common non-spherical NPs. FEM-based simulations are implemented to optimize the size, aspect ratio, concentration, and orientation of nanorods, at different positions in the perovskite layer, providing a realistic prediction of the absorption enhancement in PSCs embedding nanorods. The results show a strong dependence of the absorption enhancement on the orientation and aspect ratio of the nanorods, being the vertical orientation (parallel to the incident field) the optimal one, and an optimal aspect ratio is achieved that exceeds the absorption enhancement for the spherical NP case.

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Presentation ID: P26 *Type of Presentation: Poster*

Near Infrared Photothermoelectric Effect in Transparent AZO/ITO/Ag/ITO Thin Films

C. Bianchi[1]*, A. C. Marques[1], R. C. da Silva[2], T. Calmeiro[1], I. Ferreira[1]
[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal; [2] IPFN-IST/UL, Portugal

A new concept of oxide-metal-oxide structures that combine photothermoelectric effect with high reflectance (~80%) at wavelengths in the infrared (> 1100 nm) and high transmittance in the visible range is reported here (Fig.1). This was observed in optimized ITO/Ag/ITO structure, 20 nm of Siver (Ag) and 40 nm of Indium Tin Oxide (ITO), deposited on Aluminum doped Zinc Oxide (AZO) thin film. These layers show high energy saving efficiency by keeping the temperature constant inside a glazed compartment under solar radiation, but additionally they also show a photothermoelectric effect. Under uniform heating of the sample a thermoelectric effect is observed (S = 40 μV/K), but when irradiated, a potential proportional to the intensity of the radiation is also observed. Therefore, in addition to thermal control in windows, these low emission coatings can be applied as transparent photothermoelectric devices. [1]

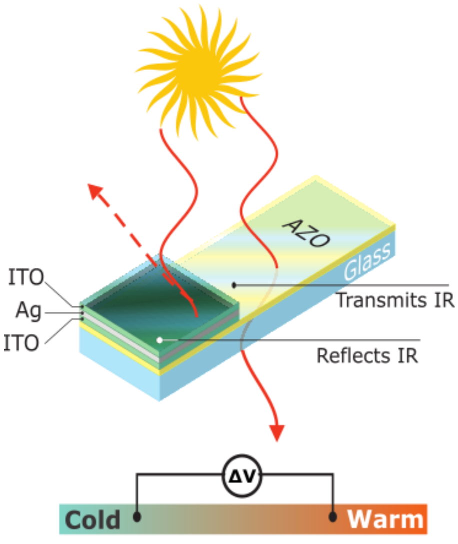

Fig. 1. Scheme of a photothermoelectric device with a oxide-metal-oxide estructure deposited on a thermoelectric thin film.

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Radiation Detection and Imaging with Micro-patterned Gaseous Detectors

F.D. Leite[1]*, A.L.M. Silva[1], L.F.N.D. Carramate[1], C.D.R. Azevedo[1], J.F.C.A. Veloso[1]
[1] *i3N, Physics Department, University of Aveiro, Portugal; *flavia.leite@ua.pt*

Micro-pattern Gaseous Detectors have received increasing attention in the scientific community during the last years and are now seen as a good alternative to other full-field detectors used in X-ray imaging systems, especially due to the accurate determination of the interaction position of each X-ray photon, as well as the energy information, making possible to perform spectral imaging with fair energy resolution and detection efficiency, at a reasonable cost [1]. This type of detectors has already been used for the elemental mapping of different samples, through X-ray Fluorescence Imaging technique, ranging from applications in the cultural heritage to the biomedical field [1], [2]; for projection and computed tomography imaging of small animals [3]; and in Compton Camera systems [4].
In this work we present the developments performed at the i3N-Aveiro in X-ray imaging systems based on gaseous detectors, both apparatus and applications, and respective results.

Acknowledgements
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Presentation ID: P28 *Type of Presentation: Poster*

Fiber-based supercapacitors for wearable electronics

J.T. Carvalho [1]*, I. Cunha[1], J. Coelho[1], E. Fortunato[1], R. Martins[1] L. Pereira[1,2]
[1]*MEON-CENIMAT/i3N, FCT-NOVA, Portugal;* [2]*AlmaScience, Campus da Caparica, Caparica 2829-516*

The sustainable development of energy storage solutions in textiles is essential to power the next generation of wearable electronics for the "Internet of Things" (IoT). This development must prioritize exploring novel alternatives that consider issues such as sustainability, reusability, repairability, and even the potential for a second-life application.[1][2] To power these devices it is essential to develop innovative and sustainable energy storage solutions with an extended lifetime, with stable cycling performances using environmentally friendly and abundant materials, not harmful, and able to result in ergonomic, flexible, stretchable, and skin or body mounted.
In this work, we explore the development of energy storage devices through different strategies, specially fiber-based 1D and 2D supercapacitors. We built 1D fiber-shaped supercapacitors (FSCs) with stretch-broken carbon fiber yarns (SBCFYs) as collectors and an in-situ regenerated cellulose-based ionic hydrogel (RCIHs) as an electrolyte. By recovering the active materials, we developed a circular process that enables the reuse and recycling of components for new 1D FSCs without compromising their electrochemical performance.[3] The electrochemical properties of SBCFYs were further improved by integrating them with pseudocapacitive materials, such as MoS_2, and using PVA/H_3PO_4 as the electrolyte, new 1D FSCs were produced.
The 2D architecture was investigated by producing supercapacitors on textile substrates. Printing techniques such as shear coating and screen-printing were employed to deposit commercially available inks including silver, carbon, and PEDOT: PSS, as current collectors and active materials. To assemble the 2D symmetric supercapacitors, we incorporate a NaCl starch and textile-based electrolyte, which provides good adhesion and maintains flexibility by forming a strong interface between the symmetric parts of the device.

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Presentation ID: P29 *Type of Presentation: Poster*

Physical and virtual sensing of lithium-ion batteries through optical fiber sensors

L. Matuck[1], V. Neto[1], J. Pinto[1], C. Marques[1], M. Nascimento[1]

[1] *i3N and Dep. of Physics, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*

The INSTABAT project is an innovative initiative aimed at monitoring key parameters of a lithium-ion battery (LiB) cells in real-time, in order to provide more accurate information about the cell's state of charge, health, power, energy, and safety to enhance the reliability, and extend the batteries life. In this way, INSTABAT intends to provide valuable insights that will improve the design and performance of LiBs, which are widely used in a variety of applications, including electric vehicles, grid storage systems, and portable electronic devices [1]. To achieve the reliable monitoring of key parameters, INSTABAT will develop four different physical (optical fibres with fibre Bragg grating (FBG) and luminescence probes, reference electrodes, and photo-acoustic gas sensor) and and two virtual sensors (electro-chemical and thermal reduced models) that will provide detailed information on the battery cell's internal dynamics. These sensors will be capable of monitoring temperature, pressure/strain, [Li^+], CO_2, absolute impedance, and potencial. The data collected by the physical sensors will be correlated with physico-chemical degradation phenomena that occur within the battery cell to identify potential areas of concern and integrated into enhanced battery management system algorithms [1].

In the scope of INSTABAT, three journal papers were already published regarding the optical fiber sensing technology and virtual thermal sensing integrated in LiB sensing. The first approached a temperature and longitudinal strain minitoring of a LiB by using FBG sensors recorded in PANDA fiber (shown in **Fig. 1 Left**) [2]. In the second paper, a study regarding the sensing of radial strain and temperature variation in a LiB (shown in **Fig. 1 Right**) [3]. In the third paper, a particle filter-based virtual sensor was developed and used to monitor simultaneously the state of charge and the internal temperature of a LiB [4].

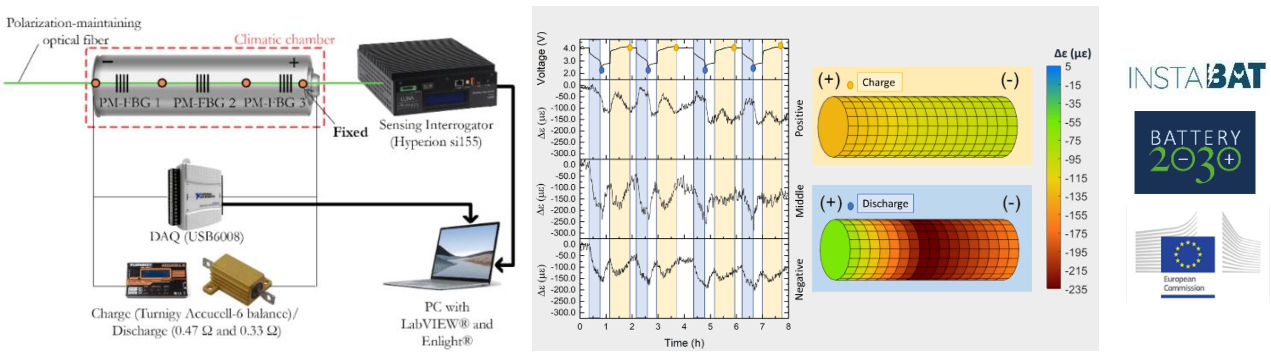

Fig. 1. (**Left**) Experimental setup for longitudinal strain and temperature tracking in a LiB [2], (**Right**) Volumetric map of radial strain variaions in a LiB [3].

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Presentation ID: P30 *Type of Presentation: Poster*

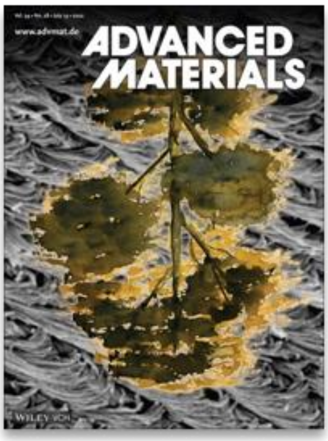
Cellulose, biomimetics, and soft functional materials

R.R. da Rosa[1]*, S.N. Fernandes[1], A. Almeida[1,2,3], P.E.S. Silva[1], P.L. Almeida[1,4], J.P. Canejo[1], M. H. Godinho[1]

[1] SBMG-CENIMAT/i3N, FCT-NOVA, Portugal; [2] LAQV/Requimte, Department of Chemistry, NOVA School of Science and Technology; [3] iBET - Instituto de Biologia Experimental e Tecnológica; [4] ISEL, IPL Portugal

Nature provides numerous structures and functionalities that inspire the development of biomimetic soft materials for various applications.

Cellulose is present in living systems and is the main constituent of the cell walls of plants. It can also be produced by bacteria (bacterial cellulose). It is a main chain polymer very much investigated due to its biocompatibility, biodegradability, sustainability, and low cost. Living systems have a close interaction with water and the presence of out-of-equilibrium systems. However, these issues, ubiquitous in nature, are still under debate needed to be addressed for cellulose-based systems. In this context, our work has been focused on the self-organization of anisotropic cellulose structures used by *Erodium* plants to disperse seeds [1].



Cellulose nanocrystals (CNCs) water suspensions are known to form liquid crystalline systems above a specific critical concentration. From an isotropic phase, tactoid formation, growth, and sedimentation have been determined as the genesis of a high-density cholesteric phase, which, after drying, originates solid iridescent films. Herein, the coexistence of a liquid crystal upper phase and an isotropic bottom phase in CNC aqueous suspensions at the isotropic–nematic phase separation is reported (Fig. Advanced Materials issue's inside back cover) [2]. The existence of an LC low-density phase is explained by the presence of air dissolved in the water present within the CNCs. The air dissolves out when the water solidifies into ice and remains within the CNCs. The self-adjustment of the cellulose chain conformation enables the entrapment of air within the CNCs and CNC buoyancy in aqueous suspensions. Bacterial cellulose hydrogels are also addressed for biomedical applications such as healing [3].

Our work also focuses on biosensors made from responsive soft anisotropic materials [4,5]. These materials take the shape of the container and are sensitive to its geometry, boundary conditions, and the presence of microorganisms, for example, *Escherichia coli* bacteria [6].

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Critical Phenomena in Complex Systems

G. J. Baxter, R. A. da Costa, S. N. Dorogovtsev, A. V. Goltsev, G. Machado, J. F. F. Mendes, G. Tímar, E. A. P. Wright, S. Yoon

TCP, i3N & Department of Physics, University of Aveiro, Portugal

We present our recent advances in the study of complex systems, with a particular focus on novel critical phenomena. The mathematical modelling of complex systems reveals significant insights into diverse applications.

A complex networks formalism provides a powerful and elegant representation of the heterogeneous interactions in a complex system. A recent focus has been on interdependent systems, which can be represented as a multi-layer structure of networks. We have discovered exotic new critical phenomena [1,2]. In the process we have developed new theoretical techniques for the analysis of complex network processes and structure [3,4]. The frequent mathematical analogies between models of different systems mean that these principles can be applied to a diversity of problems.

We describe the use of our approach in the study of epidemic spreading. We have extended the usual theoretical approach, which uses a percolation mapping, to allow for heterogeneity in interactions [5] and adapted it to allow for non-trivial initial conditions [6]. From these theoretical results, we further show how the combination of stochastic models with real-world data reveals numerous new insights into the spread of disease and the effects of policy on ongoing epidemics [7-9].

Another example of the application of our approach is the study of synchronization phenomena, and in particular the patterns of activity among neurons in the brain. The behaviour of many dynamical systems depends on the synchronization of its elements. Relatively simple oscillator models, combined with heterogeneous networks, produce a rich variety of behaviours [10]. We demonstrate the is through our recent study in which we show that a core-shell network structure in the suprachiasmatic nucleus (SCN), is sufficient to generate stable circadian rhythms [11].

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Presentation ID: P32 *Type of Presentation: Poster*

Single Electrode Yarn Shaped Triboelectric Nanogenerators for wearable applications

R. Barras[1]*, A. dos Santos[1,2], H. Águas[1], R. Igreja[1], R. Martins[1], P. Barquinha[1], L. Pereira[1,2]

[1] *AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal;* [2] *AlmaScience, Campus da Caparica, Caparica, 2829-516*

Triboelectric nanogenerators are mechanical to electric energy converter devices based on the phenomenon's of triboelectrification and charge induction. Such devices are ideal to exploit the wasted energy from natural cyclic movements of the human body, like walking. Since bendability, stretchability and wrapability are quite difficult features to achieve in planar electrical devices, fiber shape devices are the ultimate way of integrating wearables. Single electrode yarn shaped triboelectric energy nanogenerator devices (Seys-TENGs) were developed through a new method of depositing PDMS directly onto conductive carbon yarns named as in-situ curing method. Such technique allows the fast formation of a uniform thickness-controlled coating over conductive surfaces regardless of their roughness with special interest in the case of fiber shaped electrodes. Several techniques were successfully used to enhance the mechanical to electrical conversion efficiency of the Seys-TENGs namely, modification of the PDMS structure, functionalization of the CF yarns surface with ZnO nanorods, and doping of the silicone elastomer matrix using conductive chopped carbon fibers. Parameters like PDMS thickness, porosity, functionalization of CF yarns and loading content (of doping) were studied and optimized. A maximum of 72 V peak-to-peak and 10 μA (74.1 μW cm-2 of power density with a load resistance of 20 MΩ) was obtained when applying an impact force of 600 N to a set of five ZnO nanorod functionalized Seys-TENGs connected in parallel. The ZnO nanorods are intact and the output stable even after 10,000 cycles of mechanical loading at 60 N. A set of four Seys-TENGs connected in parallel are able to light at least 28 LEDs when tapping by hand, proving a contribute towards the development of basic building blocks to power the future generation of wearables.

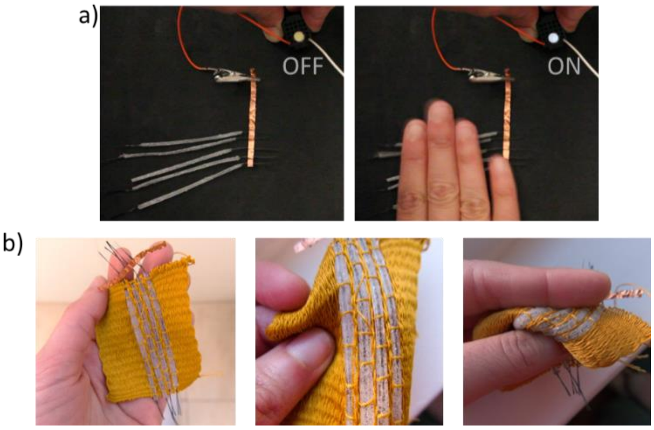

Fig. 1. a) The Seys-TENGs used to lighten an LED by taping a hand over. b) Seys-TENGs integrated on a woven structure.

Presentation ID: P33 Type of Presentation: Poster

Biodegradable luminescent QR codes based on PLA/LnMOF hybrid composites

R. Simões[1,2*], J. Rodrigues[2], J. Zanoni[2], C. M. Granadeiro[3], L. Rino[2], V. Neto[1], T. Monteiro[2] and G. Gonçalves[1]

[1] Department of Mechanical Engineering; Centre for Mechanical Technology and Automation; University of Aveiro, 3810-193 Aveiro, Portugal.; [2] Physics Department and i3N, University of Aveiro, 3810-193 Aveiro, Portugal.; [3] LAQV-REQUIMTE, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, 4169-007 Porto, Portugal. *raul87@ua.pt

Luminescent lanthanide metal-organic frameworks (LnMOFs) gathered much interest over the past decades in the scientific community due to their exceptional optical properties. There is a growing demand from producers and end-users to verify the authenticity of produced goods, guaranteeing its originality and safety status. In this scope, an anti-counterfeiting method based on a quick response (QR) code is proposed. The goal is to embed it into a product with a very specific verification procedure, using composite emissive fluorescent MOFs. The incorporation of highly emissive LnMOFs, with europium (EuMOF) and terbium (TbMOF), on a biodegradable polymer matrix of polylactic acid (PLA) was studied. The influence of the filler's concentration in the matrix's structure and the optical emission of the obtained samples was investigated in order to achieve the optimal concentration of each filler for maximum emission. The composites were fully characterized, filaments were extruded and finally 3D printed into QR codes. The optical characterization was assessed by room temperature (RT) photoluminescence (PL) and PL excitation (PLE). The results revealed that a homogeneous mixture of all the components was obtained, with no relevant structural modifications of the polymer and an excellent response to selective excitation, with well-defined intraionic lines for TbMOF @ 542 nm ($^5D_4 \rightarrow {}^7F_5$) and for EuMOF @ 615 nm ($^5D_0 \rightarrow {}^7F_2$). Hybrid composites of both fillers were also explored to create an additional encryption, obtaining different colored emission by variation of the excitation stimuli (ranging from 280 nm to 394 nm), as illustrated in Fig.1. Hence, these new luminescent composite materials can be used as traceable optical tags for a wide variety of polymeric products, capable to respond to a very specific excitation wavelength.

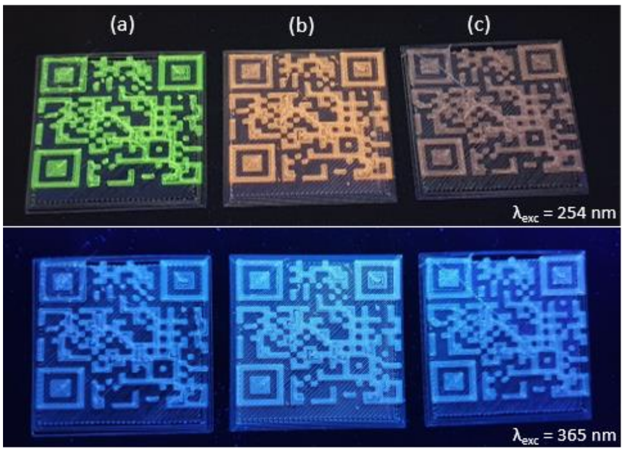

Fig. 2. QR codes with RT luminescence observed with the naked eye with UV excitation for: (a) PLA/TbMOF composite; (b) PLA/EuMOF composite and (c) PLA/TbMOF/EuMOF composite.

Presentation ID: P34 *Type of Presentation: Poster*

Intermediate Band Solar Cells based on PbS CQDs in a $MAPbI_3$ perovskite matrix

G.Ribeiro*[1],G. Ferreira[1] I. Ramiro[2], U.D. Menda[1], M. Alexandre, S. Jana, H. Águas[1] and M. J. Mendes[1]

[1] AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal;[2] Instituto de Enegía Solar, Universidad Politécnica de Madrid, Spain.

The main goal of this experimental work is the optimization of PbS Quantum Dots (QDs) for their inclusion in a high-bandgap perovskite matrix, to create an intermediate electronic band (IB)[1] in the composite semiconductor (Fig.1 (left)). This intermediate band creation can lead to a higher power conversion efficiency (PCE, up to 50% at 1-Sun illumination) of the solar cells produced. By using this nanostructured composite as an active layer, the devices can generate below-bandgap photocurrent while minimizing losses in open circuit voltage, thus generating more power via a better exploitation of the solar spectrum[2].

In this work, PbS CQD syntheses have been optimized for preferential sizes[3] ranging from 3 to 3.5 nm of particle diameter. Subsequently, peripheral ligand substitution to perovskite precursors has been developed and CQD@Perovskite composite films have been produced by spin coating. The produced films have been characterized optically, showing both absorption and emission of PbS QDs below $MAPbI_3$ perovskite bandgap, which reveals the optical signature of the intended IB nanostructured semiconductor.

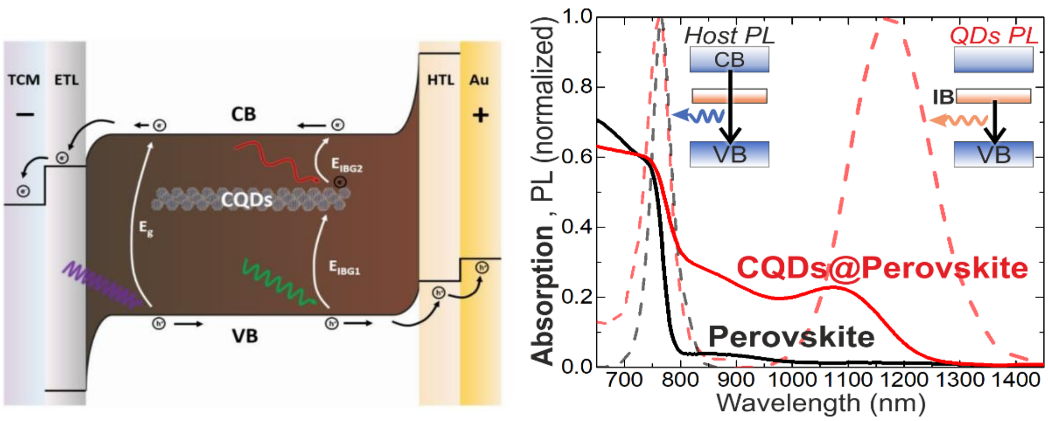

Fig. 1 (left) Band diagram schematic of a CQD@Perovskite Intermediate Band Solar Cell. **(right)** Absorption and Fluorescence Emission spectra of CQD@Perovskite compared with a $MAPbI_3$ film.

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Presentation ID: P35 *Type of Presentation: Poster*

Organic and Inorganic Solution-Processable Optoelectronic Devices

José C. Germino* and Luiz Pereira
Physics of Advanced Materials and Devices (PAMD), i3N, Department of Physics, University of Aveiro

In the last three decades, the actual renewable world has made organic/hybrid electronics in printed electronics concepts, as the new paradigm. Parallel to pure organic based, hybrid Organic/Inorganic lead-halide perovskite (HOIP) materials can be successful employed by solution-processable protocols as active layer for high-efficiency optoelectronic devices[1], such as solar cells and light-emitting diodes. In light source research, organic and perovskite LEDs (OLEDs and PeLEDs) are by far the most studied and developed materials for lighting applications, having many practical applications, particularly in displays[2]. For the big challenge in indoor lighting applications, combining two/three chromophores, trap-management, single-emitters, or tandem diodes could be used to achieve white emission (WLEDs)[3]. Although usually less efficient, all of these optoelectronic devices obtained by solution-processable protocols have a considerable cost reduction and less complex device structures. We have developed in the Laboratory of Organic/Inorganic Hybrid Electronics a series of new strategies by the usage of solution-processable protocols for organic and HOIP materials as active matrixes for achieving high-efficiency lighting (EQE ≈ 30%) and photovoltaic (PCE > 20 %) technologies. In parallel, in the field of pure Organic Photovoltaics using fullerenes as acceptors we break the efficiency record (PCE = 11.4%) in a single bulk-heterojunction layer. Finally, we hope to open the door to discussion and new possibilities for developing these kinds of devices in the energetic context of the i3N-associated laboratory and new collaborative works with our research community.

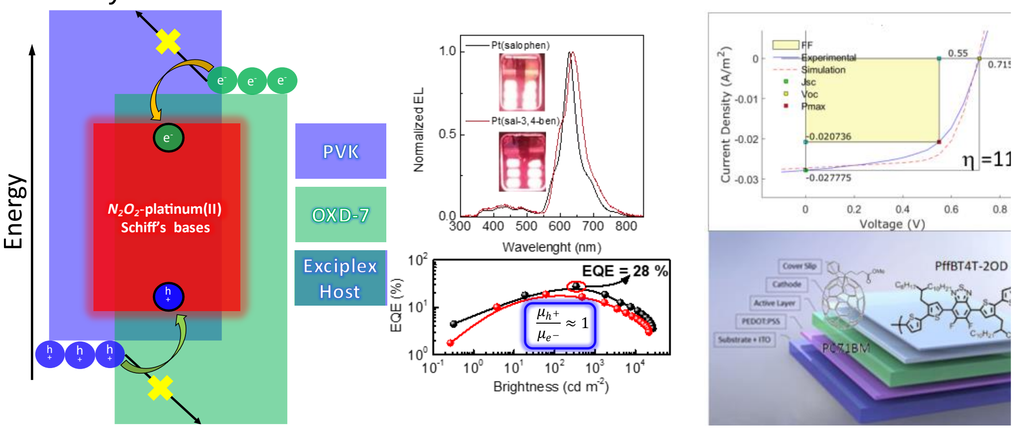

Fig. 1. Our research group's new strategies for achieving high-efficient lighting and photovoltaic devices.

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Self-aligned and Sub-µm Oxide TFTs: TCAD simulation and Fabrication

I. Santos[1]*, J. Martins[1], R. Martins[1], P. Barquinha[1]
[1] MEON-CENIMAT/i3N, FCT-NOVA, Portugal; *ìsl.santos@campus.fct.unl.pt

Oxide thin-film transistors (TFTs) have been widely employed as flat-panel display backplanes. However, their properties make them suitable for other applications in the concept of the internet of things (IoT) such as item tracking and near-field communications [1], and for implementation on large-area flexible circuitry [2]. Transit frequencies (f_T) for radio-frequency communication (13.56 MHz) cannot be met with the typically reported long channel lengths (L) and large overlap capacitances (C_{OV}) [2], [3], demanding alternative device structures and improved lithographic tools [2], [4]. This work demonstrates the development of self-aligned (SA) and sub-µm top-gate (TG) IGZO TFTs, employing doped semiconductor source/drain regions (n+ IGZO) (Fig.1). Technology Computer Aided Design tools were used to investigate on the impact of contact characteristics in device performance prior to fabrication.

SA TG TFTs with L=0.7 µm were sucessfully fabricated via direct laser writing, yieding field-effect mobilities around 5 $cm^2/V.s$, and a subthreshold slope of 0.45 V/dec. The fabricated TFTs presented small length of dopant diffusion (≈ 75 nm) and small C_{OV} (≈ 40 fF). While these devices achieved f_T of 0.1 GHz, suitable for applications such as flexible RFID. Nevertheless, distributed contact resistance of 10^{-3} $\Omega.cm^2$ hindered optimal performance, with process optimization for the n+ regions being expected to provide high performance SA TFTs.

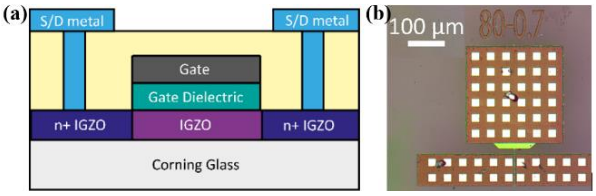

Fig. 1 Self-aligned top-gate TFTs a) shematic; b) fabricated device.

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Ce-containing bioactive glass: biocompatibility, bioactivity and antibacterial effect

S.R. Gavinho[1]*, A.S. Pádua[2], I. Sá-Nogueira[3,4], J.P.Borges[2], J.C. Silva[2], M.P.F.Graça[1]
[1] Aveiro/i3N, University of aveiro, Portugal; [2] CENIMAT/i3N, FCT-NOVA, Portugal; [3] Associate Laboratory i4HB, FCT-NOVA, Portugal; [4] UCIBIO—Applied Molecular Biosciences Unit, FCT-NOVA, Portugal; *silviagavinho@ua.pt

The dental implant has been presented several problems associated with infections that lead to the implant loss. To prevent the beginning of this conditions, implant coatings with Bioglass® have been investigated. In addition to promote bone regeneration, it is also possible to insert therapeutic ions into the Bioglass®, such as cerium. The cerium ion can improve the osseointegration, exhibit antioxidant properties and is able to prevent infectious problems associated with the dental implant placement.

In this work, 45S5 bioglass with CeO_2 in different concentrations (0.25, 0.5, 1, and 2 mol%) was synthesized by the melt-quenching. The addition of cerium presented a positive effect on biocompatibility of the 45S5 bioglass, showing no cytotoxicity for the Saos-2 cell line up to 25 mg/mL of extract concentration for all samples with cerium. The sample with 2 mol% of cerium shows an evident inhibitory effect against *Escherichia coli* and *Streptococcus mutans* bacteria. Furthermore, all samples showed the deposition of a CaP-rich layer on the surface of the material after 24 h, not compromising the bioactivity behaviour of the Bioglass® by the addition of CeO_2.

Thus, the bioglass with 2 mol% of cerium presents potential applications in bone regeneration, the filling of bone defects, or as implant coating.

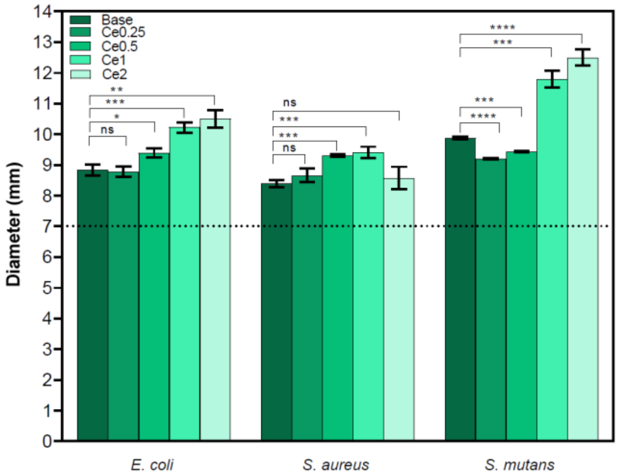

Fig. 1. Measurements of inhibition halo diameter of all samples against Gram-negative (*E. coli*) and Gram-positive (*S. aureus* and *S. mutans*) bacteria, 24 h after incubation (ns: nonsignificant; * $p \leq 0.1$; ** $p \leq 0.01$; *** $p \leq 0.001$; **** $p \leq 0.0001$).

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Presentation ID: P38 *Type of Presentation: Poster*

Analog ZTO resistive switching devices for neuromorphic applications

Carlos Silva, Jonas Deuermeier, Raquel Martins, Maria E. Pereira, Rodrigo Martins, and Asal Kiazadeh
AFMMN-CENIMAT/i3N, FCT-NOVA, Portugal

Amorphous oxide semiconductors (AOS) have been recently studied for their use in neuromorphic systems, as they are compatible with cheap, easy and low temperature fabrication processes, making them prime candidates for applications that take flexibility and transparency into account (e.g. System-on-panel applications, wearables). In this work we present three different memristor structures, all including Zinc–Tin–Oxide (ZTO) as the active resistive switching material. By choosing ZTO instead of more heavily studied AOS´s, such as Indium-Gallium-Zinc-Oxide (IGZO) (specially in display technology), we avoid the use of rare elements, resulting in a more sustainable alternative. The three different structures are compared in terms of their materials, fabrication processes, and electrical performance. Quasi-static I-V characteristics, pulse measurements analysis and synaptic performance are studied, having their neuromorphic capabilities assessed in various computational frameworks.

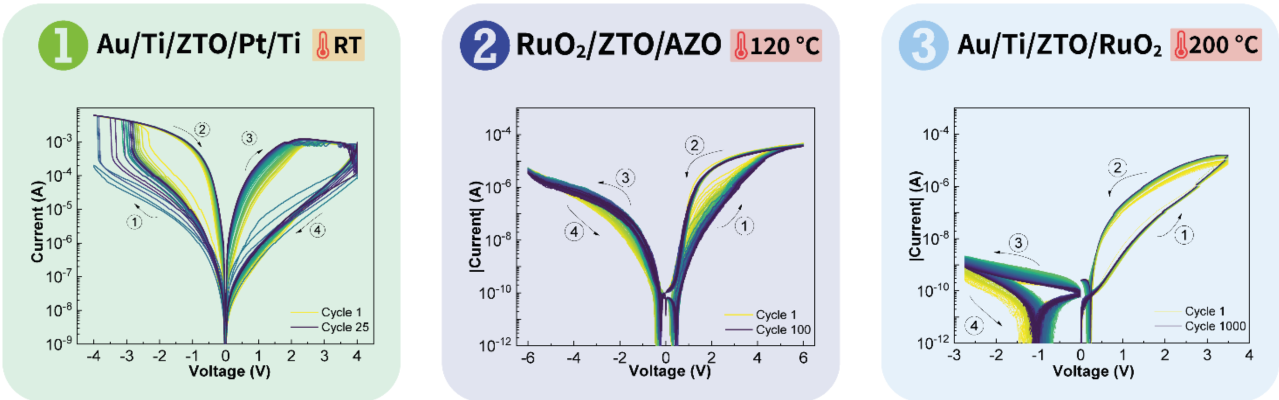


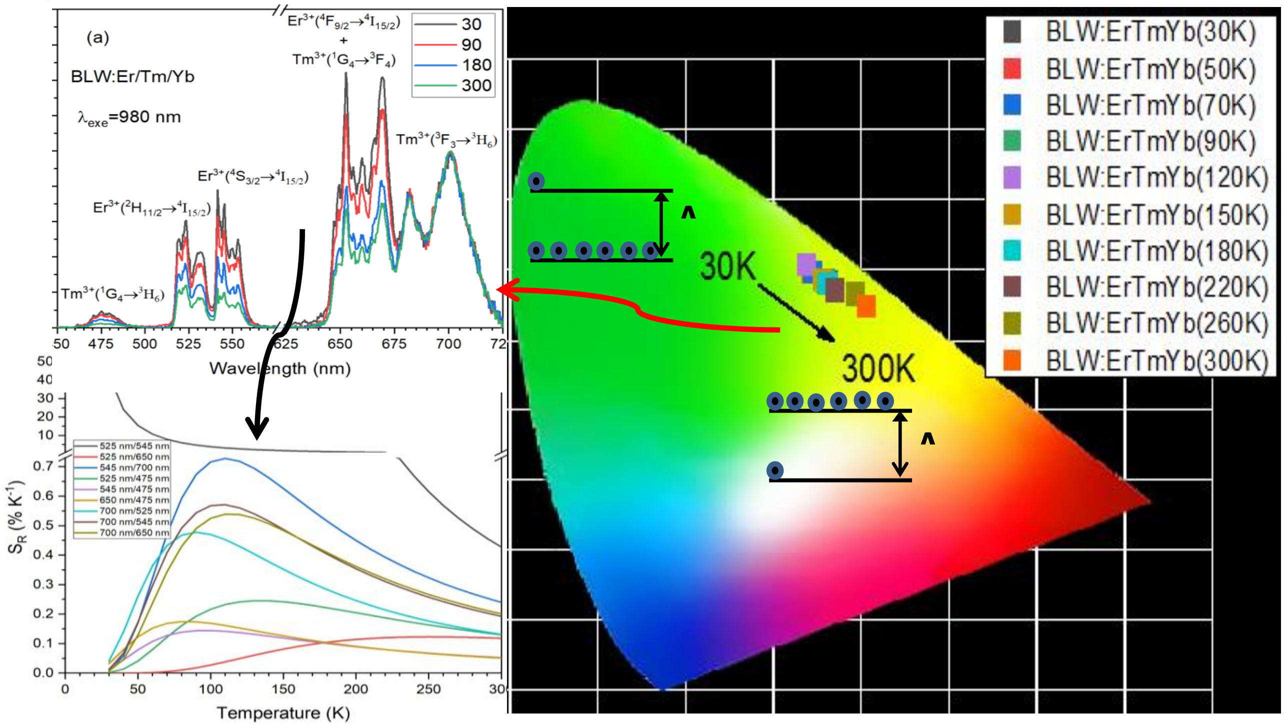
Fig. 1. I-V characteristics of the different ZTO-based memristors.

Presentation ID: P39 *Type of Presentation: Poster*

$BiLaWO_6$: $Er^{3+}/Tm^{3+}/Yb^{3+}$ phosphor: Study of multiple fluorescence intensity ratiometric thermometry at cryogenic temperatures

K. Pavani, A.J. Neves, M.J. Soares, M.P.F. Graça, S.K. Jakka
I3N & Department of Physics, University of Aveiro 3810-193, Aveiro, Portugal

Highly thermally stable $Er^{3+}/Tm^{3+}/Yb^{3+}$ tri-doped bismuth lanthanum tungstate phosphors were prepared by high temperature solid-state reaction method. The structural and morphological properties of the prepared phosphors were analysed by X-ray diffraction (XRD), Raman spectroscopy and Scanning electron microscopy (SEM) coupled with energy dispersion spectrum (EDS). Visible upconversion (UC) luminescence was measured by exciting the phosphors with 980 nm laser radiation. The dependence of the UC intensity of each emission band of Er^{3+} and Tm^{3+} ions as a function of temperature in the range from 30 to 300 K was monitored. Fluorescence intensity ratios (FIR) of thermally coupled levels (TCL) and non-thermally coupled levels (NTCL) were analysed and verified with appropriate theoretical validation. The absolute (S_A) and relative sensitivities (S_R) were esti-mated and compared with the reported systems. In the present case of $BiLaWO_6$: $Er^{3+}/Tm^{3+}/Yb^{3+}$, S_R (0.43 % K^{-1}) related to TCL of Er^{3+} UC is found to have maximum sensitivity compared to any of the NTCL combinations at 300 K. From this study we inferred that the S_R values estimated from NTCL are smaller than that of TCL involved in BLW: $Er^{3+}/Tm^{3+}/Yb^{3+}$ phosphor. The temperature dependent CIE color coordinates were also evaluated in the cryogenic temperature region.



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Self-Powered Security Tag based on Polypyrrole-cellulose composite for next-generation IoT

G. Ferreira[1], S. Das[2], S. Goswami[2], Luís Pereira[1,2], R. N. Pereira[3], R. Martins[1,2], E. Fortunato[1,2], S. Nandy[*,1]

[1] CENIMAT/i3N, FCT-NOVA and CEMOP/UNINOVA, Caparica, Portugal,[2] AlmaScience Colab, Madan Parque, 2829-516 CAPARICA, Portugal, [3] Department of Physics and i3N - University of Aveiro, Portugal, *s.nandy@fct.unl.pt (SN)

It is of paramount importance that mankind advances towards green and sustainable technologies, cutting down e-waste, and concurrently not neglecting the fast upgrading of the digitalization state-of the art. In this context, paper or cellulose substrate have a great impact as promising materials towards the shift of ecological alternatives. The present work is fully committed to finding viable options to replace some of the materials commonly used in electronic devices, most of them expensive or unsustainable, compared to paper, due to its recycling properties and availability. The development of cellulose-based matrices and their functionalization with conductive polymer to produce devices capable of harvesting energy of the electric energy generated by a mechanical stimulus was targeted. [1,2] It instantaneously generated an electrical signal of 0.91 W m^{-2} due to a mechano-responsive charge transfer mechanism. Apart from using conventional electrode materials, graphite pencils were also utilized towards a more simple, environmentally friendly and cost-effective approach. Furthermore, different arrays of TiPP have been designed to create a unique coding system (high/low signal) that can simultaneously enable self-powered sensing and an identification system. (Fig. 1.) This is exhibited by a rapid but simple signal processing method used in several applications like R-G-B color codes, personal ID cards and product identification tags. A straightforward signal processing circuit that includes an effective simulation, was also demonstrated to validate the working principle of such self-powered security identification tags. [3]

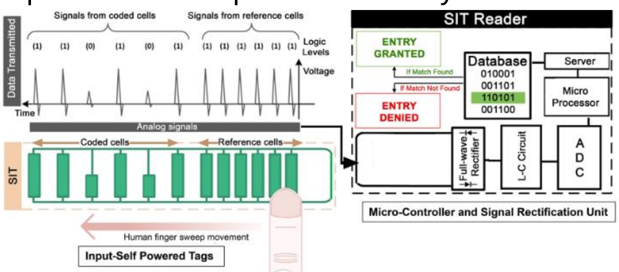

Fig. 3. - Generalized flow diagram on how the self-powered electronic tags are taken as input and the various steps involved in processing those signals so that an application can be create

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