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Book of Abstracts

Contents

Advanced materials and processes for Energy / 1

Ferroelectricity in nanoscaled ZrO2 thin films and their promising application in energy storage capacitors

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Zirconia and hafnia based thin films have attracted considerable attention in the last decade due to the existence of a ferroelectric behavior at the nanoscale, which can enable the downscaling of the next-generation of non-volatile memory and energy storage devices [1,2].
In this presentation an overview regarding the recent advances on these materials will be given [2]. Then, our most recent results on this topic will be discussed. The effect of the insertion of a thin dielectric HfO2:Al2O3 (HAO) layer, with a thickness ranging from 2 to 8 nm, on the tunability of the ferroelectric and energy storage characteristics of ZrO2 films is presented [3]. An optimal combination of high energy density of 54.3 J/cm3 and good storage efficiency of 51.3% is obtained for the ZrO2 film capacitors with a 2 nm-thick HAO insert layer. These values correspond to an increase of ˜ 55% and ˜ 92%, from the respective values of pure ZrO2 film capacitors. Moreover, special attention will be given to the existence of a novel rhombohedral R3m phase in ZrO2 thin films [4]. This presentation relates experimental structural studies to density-functional theory (DFT) calculations to disclose this novel rhombohedral R3m phase in epitaxially-strained (111)-oriented ZrO2 thin films, grown by ion-beam sputtering deposition technique on (111)-Nb:SrTiO3 substrates. Comprehensive local and macroscopic ferroelectric characterization reveals that these ZrO2 films display a switchable ferroelectric polarization reaching 20.2 μC/cm2 with a coercive field of 1.5 MV/cm. Interestingly, these films show a wake-up free ferroelectric behaviour.

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Advanced materials and processes for Energy / 2

Solid polymer electrolytes for solid-state lithium-ion batteries: Challenges and opportunities for the next generation of energy storage

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The modern world is facing a growing number of interconnected electronic devices in the scope of the Industry 4.0 and Internet of things concepts. As the technology develops and the devices get smaller, lighter and portable, the need for more efficient storage systems capable of powering these devices arises as a critical challenge. Despite their widespread use and strong position as leader in this market, lithium-ion batteries face significant issues when it comes to safety, performance and environmental impacts, that must be addressed to as soon as possible. Several possibilities, as self-healing and shutdown functions, the implementation of additive manufacturing techniques, beyond

lithium technologies and solid-sate batteries are being intensively studied in order to address these issues.
Solid polymer electrolytes (SPEs) are expected to represent a solution for the issues present in conventional lithium-ion batteries, as they have the potential to be more durable and safer than the commonly used separator/electrolyte systems. However, there are still relevant scientific challenges to be addressed in order to meet the performance requirements needed for application, in particular at the level of room temperature ionic conductivity.
This presentation will present a brief overview on the recent advances in solid-state lithium-ion batteries with particular focus on the three-component approach for SPEs development. This approach allows a fine tuning of the SPE properties through the use of two distinct and complementary fillers. In particular, the application of micro and mesoporous materials (MOF-808, clinoptilolite, MFI, ETS-4) as passive fillers, complemented with ionic liquids ([BMIM][SCN], [EMIM][TFSI], [BMIM][N(CN2)]) for improving the ionic conductivity shows promising results, with suitable room temperature ionic conductivity (1.9×10-4 S.cm-1) and excellent battery performance (160.3 mAh.g-1 at C/15) over prolonged charge/discharge cycles.

Advanced materials and processes for Energy / **3**

Materials and Processes for Energy at C2TN: an Overview

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An overview of the activities made at C2TN in the thematic line of the Advanced Materials and Processes for Energy will be presented. Special emphasis will be given to the main activities made in this area at C2TN, in particular in the fields of thermoelectric materials and technology, as well as in intermetallics for hydrogen storage, biofuel production by organic materials irradiation and novel nanostructured nuclear fuels.

Quantum Materials and Quantum Technologies (Posters) / **4**

Quantum dot PL emission control through a nearby graphene layer

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The transfer of energy from semiconductor Quantum Dots (QDs) to Graphene in hybrid structures provides a rich environment to explore excitation dynamics in heterogeneous hybrid systems The photo-physical properties of QDs can be predictably fine-tuned by size selection, and Graphene can also be doped, with the aim of producing well-defined conditions for photoexcitation and energy transfer. Additionally, both Graphene and QDs display superior photo-stability. For all these reasons, hybrid QD-Graphene superstructures have strong potential for use in a wide variety of photonics applications where a well-defined modulation of optical and spectroscopic properties are crucial [1]. For example, several works have already demonstrated the use of graphene as a substrate to manipulate and quench photoluminescence (PL) [2], to enhance resonance Raman signals [3], or to support saturated absorption mode-locking of ultrafast lasers [4].
Here we explore the changes in the PL emission of CdSe colloidal QDs deposited on CVD graphene as the Fermi-level of graphene is varied. In solution, QDs'PL spectrum consists of a band centered at λ=590 nm and FWHM of about 40 nm. The emission band becomes considerably narrower as

the doping level of graphene is increased. Furthermore, the emission maximum shifts to the blue when switching from p- to n-type doping of the graphene. We suggest that the reason is selective quenching of the emission of some QDs within the size distribution. Charge transfer from graphene to a QD via tunneling can be possible when the Fermi energy of graphene is higher than the first energy level of QD electrons. Shifting graphene Fermi level allows us to control the amount of charge carriers available to be transferred via tunnelling to a subset of QDs within the size distribution.
The theoretical part of this work is divided in two parts. The first one is dedicated to the evaluation of the tunneling transition probability using Bardeen's. We found that the tunneling probability is quite low (˜1 s-1) due to a large wave-vector mismatch between the QD electronic states (near the Γ point) and graphene's Dirac point. Even though, QDs and graphene will come to an equilibrium within a few seconds after being put in contact. The second part focuses on the statistics of electrons in the system at equilibrium, which allows us to evaluate the occupation probability of the QD lowest level in the conduction band and the fraction of QDs that cannot be excited by light because of the Pauli blocking and, therefore, do not contribute to the PL emission. It explains the QD PL spectrum dependence on the graphene Fermi energy.

Quantum Materials and Quantum Technologies / 5

Materials science aspects of quantum colour center creation in diamond by means of ion implantation

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Colour centers in diamond are in the focus of interest as single photon emitters for quantum (Q) technologies. Q metrology has already been demonstrated using the nitrogen-vacancy NV– center, which has the crystal symmetry C3. However, defects with D3d mirror symmetry, such as the group IV centers [1] SiV, GeV, SnV and PbV, but also MgV, show optical properties superior to NV, and are envisaged for single photon Q communication.
The D3d symmetry is the result of the impurity occupying a lattice site in the center of two vacancies, the so-called split-vacancy configuration as shown in Fig. 1 (bottom).
The most widely used method to create the colour centers is ion implantation. Here one is faced with the challenge to maximize the fraction of implanted impurities in the split-vacancy configuration and to minimize structural damage resulting from ion implantation in order to achieve a narrow spread of optical properties of the centers.
We present results on the lattice location and confocal PL measurements of radioactive 121Sn in diamond [2], where we could unambiguously show that, following annealing at 920℃, »30% of implanted Sn is found in the split-vacancy configuration. Confocal photoluminescence (PL) revealed the characteristic SnV– line at 621 nm, with an extraordinarily narrow ensemble linewidth (2.3 nm) of near-perfect Lorentzian shape.
We are currently addressing colour center creation within a collaboration that includes KU Leuven

Quantum Solid-State Physics (Belgium), University of Torino (Italy), and Universidade de Aveiro. Emission channeling (EC) lattice location experiments using the radioactive isotopes 121Sn, 209Pb, 27Mg, 45Ca and 89Sr are performed at the CERN-ISOLDE facility, while PL characterization of diamond samples implanted with stable isotopes (at KU Leuven or ISOLDE) takes place at the Universities of Torino and Aveiro.

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Advanced Materials and Processes for Energy (Posters) / **6**

Nuclear microprobe: the tool to characterize new materials for energy conversion

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The ion beam analytical (IBA) techniques capabilities are enhanced when coupled to a scanning nuclear microprobe due to the possibility of: i) focusing the beam to sub-micrometer spot sizes and, ii) rastering the area under analysis. In this way, it is possible to obtain elemental distribution maps and the elemental depth profile in a fully quantitative manner.

The type of materials characterized in the nuclear microprobe installed at CTN-IST is vast and includes, among others: biological, alloys, cultural heritage or semiconductor materials.
In this work, we will focus on two materials used to convert the sun light into electricity: perovskites and CIGS (CuIn1-xGaxSe2) materials.

Optoelectronic defects, such as composition inhomogeneities created, for example, during the manufacturing process, can be revealed during the characterization (fig. 1).

Examples using different type of beams (protons or alpha particles) and energies (up to 2 MeV) will be given to show the capabilities of the IBA techniques and the nuclear microprobe in the this field.

Quantum Materials and Quantum Technologies (Posters) / **7**

Spectrum of very excited flux tubes in SU(3) gauge theory

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As gluons, the force carriers of strong interactions, have color charge; the gluonic field is squeezed in space-time due to the self interaction and forms a flux tube in the vacuum; this is in contrast to the electromagnetic field spreading out in space. The dominant behavior of the flux tube is string-like, hence, it can be modeled with a thin relativistic string. The quantization of the string leads to a tower of levels. The simplest model of a quantum string is known as the Nambu-Goto string model. We study the spectrum of the flux tubes between quark and antiquark for pure SU(3) gauge using lattice

QCD in 3+1 dimension. We could get a significant number of excitations for different symmetries of the flux tube. To accomplish this goal, we used a large set of appropriate operators, different lattice QCD actions besides smearing techniques and solving generalized eigenvalue. Moreover, we compare our results with the Nambu-Goto string model to see the deviation from it, which could be a signal for novel phenomena beyond the model.

Materials and technologies for Health and Environment (Posters) / 8

Design and characterization of new membrane housings for Portable Hemodialysis Devices

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Patients with end stage renal disease (ESRD) are progressively increasing and the demand for renal replacement therapies is expanding [1]. Transplantation is the most effective option, but it is limited by the scarcity of organs thus making in-center hemodialysis (HD) the most reliable form of therapy. The crucial role of HD dosage in critically ill patients suffering from ESRD is well established. Studies show that higher frequency HD not only increases the quality of life of ESRD patients but also lowers morbidity and mortality rates [2]. Novel microdevices designed to perform continuously will result in a smoother correction of uremic abnormalities and offer greater mobility for ESRD patients. Early development of a portable artificial kidney (PAK) for the treatment of ESRD is envisioned based on a novel blood purification device that integrates membrane technology in a microfluidic system –the microfluidic membrane device (MFMD).
Medical applications for 3D printing are expanding rapidly and are expected to revolutionize health care [3]. Actual and potential applications include tissue and organ fabrication, customized prosthetics, anatomical models, implantable and extracorporeal artificial organs [4]. This work focuses on the design and fabrication of membrane housings with well-defined microfluidic flow channels using 3D printing technology.
The device was designed using Onshape®, a 3D CAD (computer-aided design) software, and fabricated using a 3D printer (Ultimaker2+, Netherlands), using acrylonitrile butadiene styrene (ABS). The device was connected to an in-house built experimental system that simulates the extracorporeal blood circulation circuit found in HD machines and is capable of measuring very low pressure variations (< 1 mmHg) under dynamic conditions.
In order to characterize the membrane housings in terms of channel height, residency time, total volume and shear stresses at the wall of the device, experiments using pure DI water were performed by placing a non-permeable polyester transparency film in the place to be occupied by the HD membranes in the future (like shown in Figure 1).
Results show that both channels were approximately 100 μm in height and that flow rates between 14 and 60 mL/min impose shear stresses between 6.3 and 27.8 Pa.

Materials and technologies for Health and Environment / 9

Development of novel monophasic hybrid membranes for improved artificial kidney devices

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Hemodialysis (HD) is a clinically well-established membrane-based treatment for blood purification under extracorporeal blood circulation. Most of the hemodialyzers/artificial kidneys on the mar-

ket are composed of synthetic polymer membranes with large pore sizes that allow the removal of uremic toxins (UTs) of large molecular weight. Nevertheless, these membranes are hydrophobic by nature and must be rendered hydrophilic before they can be used to filter blood toxins, thus adding an extra step in the preparation process. Even though they are able to remove many UTs from the blood of end stage renal disease (ESRD) patients, over 50% of known UTs remained untouched. Furthermore, they have been linked to the convective removal of useful and even vital compounds found in blood [1], [2].
Cellulose is a low-cost natural polymer and one of the most abundant renewable organic materials and cellulose acetate (CA) membranes are extensively used for their great mechanical flexibility, accurate chemical selectivity, and film-forming properties which allow the synthesis of membranes which cover a wide range of membranes processes, from ultrafiltration (UF) to reverse osmosis (OS). CA membranes also have great potential for artificial kidney devices, however disadvantages such as poor mechanical strength, low chemical resistance and thermal stability must be addressed. To overcome these limitations, we have developed monophasic hybrid cellulose acetate silica (CASiO2) membranes, with silica (SiO2) contents between 5 and 18 wt% by an innovative method which combines sol-gel and phase inversion techniques [1], [3].
The morphological and topographical characterization of the CASiO2 membranes was performed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Static contact angles were measured through the sessile drop method and permeation experiments were performed to determine the hydraulic permeability and rejection coefficients to reference solutes pertaining to the metabolic functions of the kidney [3].
SEM confirmed asymmetric membrane cross-section structures and AFM showed that the introduction of SiO2 reduced the submicron surface roughness when compared to the pure CA membrane. Contact angles revealed that the wettability increased for membranes containing high wt% of silica. Permeation studies show that the incorporation of SiO2 into CA membranes increased the hydraulic permeability of the CASiO2 membranes and that all hybrid membranes fully permeated urea and completely rejected albumin. Regarding the hemolysis assay, all CASiO2 membranes were non-hemolytic, low thrombogenic and did not promote the highest stages of platelet activation [3].

Scientific Area:

Materials and technologies for Health and Environment (Posters) / 10

Characterization of a cellulose acetate-based monophasic hybrid membrane under dynamic conditions: towards improved blood purification devices

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Chronic kidney disease, a growing public health concern affecting 11-13% of the global population is defined by an irreversible worsening of renal function which can lead to end stage renal disease (ESRD) [1]. Hemodialysis (HD) is the most widely used renal replacement therapy to purify the blood of ESRD patients and the majority of hemodialyzers on the market are composed of synthetic polymer membranes with large pore sizes that allow the removal of uremic toxins (UTs) of large molecular weight. Nevertheless, studies focused on the ultrafiltrate removed from ESRD patients identified the convective removal of useful and even vital compounds found in blood [2]. In this study, a novel cellulose acetate-based monophasic hybrid skinned amine-functionalized CA-SiO_2-$(CH_2)_3NH_2$ membrane was synthesized by an innovative method which combines the phase inversion and sol-gel techniques [3,4]. The morphological characterization of the hybrid membrane was performed by scanning electron microscopy (SEM) and the chemical composition was analyzed by Fourier transform infrared spectroscopy in attenuated total reflection mode (ATR-FTIR). Characterization of the monophasic hybrid CA-SiO_2-$(CH_2)_3NH_2$ membrane in terms of permeation properties was carried out in an in-house built single hemodialysis membrane module (SHDMM) under dynamic conditions. Permeation experiments were performed to determine the hydraulic permeability (Lp) and rejection coefficients to reference solutes pertaining to the metabolic functions of the kidney

and determination of the molecular weight cut-off (MWCO). For comparison purposes, a pure cellulose acetate (CA) membrane was also synthesized and characterized. SEM confirmed asymmetric membrane cross-section structures and ATR-FTIR confirmed the covalent bonding between CA and SiO2. The permeation studies revealed for the novel anime-functionalized membrane an increase in the hydraulic permeability by an approximate factor of 2 when compared to the pure CA membrane. The two membranes under study showed to be fully permeable to small water-soluble uremic toxins, while retaining BSA. CA-SiO_2-$(CH_2)_3NH_2$ and pure CA membranes yielded an estimated MWCO of 24.5 kDa and 18.1 kDa, respectively.

Advanced Materials and Processes for Energy (Posters) / 11

Tetrahedrite co-doping with Se and Ni or Cr for thermoelectric applications

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Currently available commercial thermoelectric generators contain expensive and potentially hazardous elements, such as Bi, Pb or Te. To overcome this hindrance, the application of alternative materials, like the p-type semiconductor mineral tetrahedrite (Cu12Sb4S13), is being studied. Tetrahedrite is a naturally occurring and abundant mineral with low toxicity that displays good electrical and thermal properties, with a figure of merit, zT, of 0,6 at 700K. Comparatively to commercially available thermoelectric materials (zT>1,0), tetrahedrite still has a small zT, but various studies suggest that it can be increased via isovalent doping. [1]
The objective of this project is to study the effect of selenium (Se) and nickel (Ni) or chromium (Cr) simultaneous isovalent doping in the thermoelectric properties of tetrahedrite. Powder X-Ray Diffraction, Raman Spectroscopy and Scanning Electron Microscopy, with Energy Dispersive Spectrometry, were used in the characterization of Cu12-xMxSb4S13-ySey, (M= Ni or Cr). After annealing at 723K for 7 days (the current stage of the production process), the samples show a main tetrahedrite phase (with the lowest ≈84% molar content), and a minor presence of secondary phases. Measurements of the Seebeck coefficient and electrical resistivity, suggest that doping improves the power factor, with the Cu11,5Ni0,5Sb4S12,5Se0,5 sample achieving the highest value of 1277,73 μW/m.K2 at 300K. After estimation of thermal conductivity with the Friedman-Franz law, a figure of merit zT=0.32 at 300K (Fig. 1 and 2) was obtained.

Advanced materials and processes for Energy / 12

A Quest To The Optimal Contact Fixation Technique For Manganese Doped Tetrahedrites

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Thermoelectric generators (TEG's) are devices able of converting waste heat into usable electricity through the Seebeck effect, which makes them very attractive to fight against global warming. To develop novel TEG's, made of more sustainable, cheap, and less toxic materials, many crucial aspects need to be considered. The nature and quality of the interface between the TE materials and the solders/electric connectors used on the device are some of them. High electrical and thermal interfacial resistivity ruin the devices performance, even if materials with good thermoelectric properties are used.
In this work, several jointing fabrication techniques are explored to evaluate the optimal method to connect manganese doped tetrahedrite legs to copper contacts. To build the thermoelectric legs, Cu11Mn1Sb4S13 tetrahedrites were synthesized by solid state reaction and hot-pressing techniques. The materials where shaped into cubes and connected to copper electrodes manually and using cold and hot-pressing techniques. Nickel paint, water-based Ag paint, and a Zn-Al5wt% solder, were used for materials jointing, being also explored the possibility of contact fabrication without the use of any paints or solders.
The contact resistance of the legs/contacts joining was measured on a custom-made system based on a three-contact pulsed current method and computer simulations using the COMSOL Multiphysics program were made. The simulations consisted of a thermoelectric couple made by a tetrahedrite leg (p-type semiconductor), and a magnesium silicide leg (n-type semiconductor). A 603 K thermal gradient and electrical insulation conditions were applied to an optimized model [1]. For the simulations, some of the measured contact resistance values were used and the impact on the performance of the thermoelectric couple was evaluated by obtaining the respective I-V and I-P curves.

Advanced Materials and Processes for Energy (Posters) / 14

Synthesis, characterization and thermoelectric properties of intermetallic compounds

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Thermoelectric materials are important for power-generation devices that can convert waste heat into electrical energy. This conversion may have an important role in the current challenge for the development of alternative energy technologies.
In the present work, the intermetallic thermoelectric materials with the formula RCu9Sn4 (R=Nd, Pr, La, Y) and their stoichiometric variations RCu9.4Sn3.6 have been first prepared and studied. The initial purpose of the work was to obtain tetra-cage materials in which the phenomena of rattling (oscillation of the central atom) is observed. This is expected to decrease the thermal conductivity, therefore increasing the final thermoelectric efficiency of the material. The materials were synthesized by arc melting and subsequently annealed. The heat treatments were carried out using the following sequential procedures: the annealing first lasted 21 days at 680 ℃, followed 10 days at 800 ℃. X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) were combined to characterize them. The analysis indicated that it was not possible to obtain monophasic samples before or after the thermal treatments. However, the treatments led to the formation of a novel phase for the Y and Nd samples, in course of characterization. An interesting point is that the secondary phase Cu3Sn was observed in all samples, in some with a significant percentage. The thermoelectric properties (electrical resistivity and Seebeck coefficient) were subsequently studied, but the results showed a low Seebeck coefficient for these materials.
Subsequently, the CeMSn (M = Cu, Ni) materials were prepared and studied. The work shifted to this family of compounds because they possess a high peak near the Fermi level in their Density of State (DOS). This is very interesting because the point at which the Fermi level intersects the DOS is related to the value of the Seebeck coefficient. In particular, the greater the slope at the point of intersection, the greater can be the value of the Seebeck coefficient. For this reason, samples have been synthesized by slightly varying the stoichiometry, Ce:M:Sn, to 1-0.9-1.1 and 1-1.1-0.9, to change the Fermi level. These samples were also synthesized by arc melting and annealing (10 days at 800 ℃). Characterization with XRD and SEM proved some of them to be monophasic, a fundamental feature for a proper study of physical properties. Further studies will assess thermoelectric

properties.

Materials and technologies for Health and Environment (Posters) / 15

Magnetoliposomes based on magnetic/plasmonic nanoparticles loaded with new antitumor drugs for combined cancer therapy

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Cancer is one of the main public health problems and the World Health Organization (WHO) points it as the second leading cause of death in the world [1]. Stimulus-responsive nanosystems have been a promising approach to control the release and delivery of therapeutic agents to target sites. In this work, manganese ferrite nanoparticles were decorated with gold nanoparticles or covered with a gold shell. These magnetic/plasmonic nanostructures were entrapped in liposomes for application in dual cancer therapy [2], combining chemotherapy and photothermia. The magnetic/plasmonic nanoparticles were characterized by XRD, UV/Vis. absorption, HR-TEM and SQUID, exhibiting a superparamagnetic behavior at room temperature. The average size of the gold-decorated nanoparticles was 26.7 nm for MnFe2O4 with 5-7 nm gold nanospheres. The average size of the core/shell nanoparticles was 28.8 nm for the magnetic core and about 4 nm for the gold shell.
Two new promising antitumor drugs (tricyclic lactones), active against colorectal adenocarcinoma and non-small cell lung cancer, were loaded into these nanosystems with very high encapsulation efficiencies (over 98%). Assays on human tumor cell lines have shown that these nanocarriers do not release the antitumor drugs in the absence of irradiation. Furthermore, the nanosystems have no effect on the growth of primary (non-tumor) cells (with or without irradiation). Drug-loaded systems containing the core/shell magnetic/plasmonic nanoparticles efficiently inhibit tumor cell growth when irradiated with red light (article submitted), being suitable for a triggered release promoted by irradiation.

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Quantum Materials and Quantum Technologies / 16

Symmetry-induced even/odd parity in charge and heat pumping

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It is shown that the presence of discrete symmetries in Floquet systems connected to metallic reservoirs imprints a definite parity on the charge and heat pumping as a function of the reservoir's chemical potential, μ. In particular, when particle-hole symmetry (PHS) holds, the pumping of charge (heat) is an odd (even) function of μ. Whereas, if only the product of PHS and parity symmetry is present, pumping of charge (heat) is even (odd) in μ. Our results also extend to the presence of other unitary symmetries and provide a simple criterion for reversing (or maintaining) the direction of the flow. We illustrate our findings using two variants of the Su-Schrieffer-Heeger model under a time-periodic perturbation.

Scientific Area:

Advanced Materials and Processes for Energy (Posters) / 17

Growth of Ruddlesden–Popper Ca3Mn2O7 thin films by Pulsed-Laser Deposition

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Naturally Layered Perovskite structures with improper ferroelectricity [1, 2], such as the Ruddlesden-Popper calcium manganite compound Ca3Mn2O7, offer an alternative route to achieve non-expensive and high-performance room temperature multiferroic magnetoelectricity for information storage, sensors, and actuators or low power energy-efficient electronics. They allow exploring oxygen octahedra nonpolar rotations and cation site displacement to attain non-centrosymmetry. Additionally, due to their high sensitivity to lattice-distortions, their preparation in thin film form over crystalline substrates allows the manipulation of acentricity and enables the tuning of lattice, electric and magnetic interactions. However, the preparation conditions to obtain the Ca3Mn2O7 phase with the Ruddlesden-Popper structure need to be optimized and their properties have not yet been explored. As such, thin films of Ca3Mn2O7 have been prepared over SrTiO3 substrates by Pulsed Laser Deposition, using a Ca3Mn2O7 target. Polycrystalline Ca3Mn2O7 was synthesized using a convention-al high-temperature ceramic route. The structural studies show that in the films prepared on SrTiO3, at 730 ºC, with 4 J/cm2 laser fluence, 10-3 mbar oxygen pressure and with a post-annealing process, the Ca2Mn3O7 phase is stabilized, as confirmed by XRD and Raman Spectroscopy. The corresponding EDS analysis further gives a Ca/Mn atomic ratio of ˜1.5:1, consistent with the presence of this phase. The magnetic properties were measured using a SQUID magnetometer, showing an antiferromagnetic transition at 110 K. The dielectric properties of the films show a relaxor-type behavior. The Havriliak-Negami function was fitted to the real and imaginary permittivity as a function of frequency (Fig. 1). The dielectric properties of the films will be discussed and presented, highlighting the phase evolution and stabilization in the films.

Materials and technologies for Health and Environment (Posters) / 18

99mTc-labeled L/D-amino acids for cancer imaging

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Radiolabeled amino acids for assessment of increased rates of amino acid transport in cancer cells continue to gain importance in cancer imaging. Radiotracers targeting transporters of cationic amino acids (CAs), such as Cationic Amino acid Transporter-1 (CAT-1) and Amino acid Transporter B^{0,+} (ATB^{0,+}), hold great potential as imaging biomarkers for predicting and monitoring response to arginine deprivation therapy or imaging brain tumors, among other applications. Interestingly, nearly no metal-based radiotracers based on CAs are known, especially those containing radiometals obtained from widespread commercially available generators such as technetium-99m (^{99m}Tc) or gallium-68 (⁶⁸Ga). Therefore, aimed at addressing unmet needs in the clinical setting and within the framework of a FCT-funded project (Targeting the transporters of cationic amino acids for cancer radiotheranostics: experimental and computational chemistry approach), we have proposed the design of new families of ^{99m}Tc-labeled cationic L/D-amino acid derivatives and the evaluation of their internalizing properties in representative cancer cell lines. For the most promising complexes, we will further assess their biological behavior in adequate animal models.
Herein, we will describe the synthesis and characterization of L/D-amino acid (Arg, Lys, His and Trp) containing chelating ligands, as well as the radiosynthesis of the corresponding ^{99m}Tc complexes.

Materials and technologies for Health and Environment (Posters) / 19

Chewing simulator studies on leucite reinforced with zirconia for dentistry

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Among ceramics, zirconia is one of the most used material to repair/replace damaged/lost dental tissues, due to its high toughness [1]. Glass veneers are usually applied over zirconia frameworks to improve their optical properties [2], but they generally result into chipping [3], leading to extensive wear of the antagonist teeth. Leucite and lithium disilicate are alternative materials to be used without the application of a coating due to their excellent aesthetic properties. However, they present low toughness and therefore fracture and extensive wear of the antagonist teeth and the prosthetic material may occur [4]. Thus, this work aims to develop leucite reinforced with 25 wt% of zirconia nanoparticles in order to improve tribological behavior. The performance of the produced material was compared to that of 100% leucite and 100% zirconia. All samples were produced by unidirectional compressing, followed by sintering at 1000ºC for 6h (75% and 100% Leucite) and 1500ºC for 2h (zirconia). The samples'mechanical properties were characterized and their tribological behaviour against natural human cusps using a chewing simulator was accessed. The results show that the reinforcement with 25% zirconia reduced the prosthetic materials'wear when compared to 100% Leucite. Regarding wear mechanisms, mild abrasion was observed for the composite (Figure 1B) while for 100% leucite fracture occurred with the spalling of large quantities of material (Figure 1A). In addition, a reduction of dental wear was observed for 75% Leucite when compared to 100% Leucite, being similar to that observed for 100% zirconia. The cusps against 100% Leucite showed abrasion, delamination and fracture (Figure 1C), while the cusps against the composite presented mainly abrasion (Figure 1D).
Overall, the present results are promising, since the wear of the antagonist teeth is much lower than that observed with 100% Leucite, being close to the one obtained with 100% zirconia.

Quantum Materials and Quantum Technologies / **20**

Quantum digital simulation of the time evolution of quantum systems in the NISQ era

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In this poster, we will explore the principles of quantum digital simulation of the time evolution of quantum systems.

Scientific Area:

Welcome session / **21**

LaPMET-Laboratory of Physics for Materials and Emergent Technologies

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In this presentation we will give a short overview of the pathway of the associate laboratory LaPMET-Laboratory of Physics for Materiais and Emergent Technologies, from the initial idea to to the underway implementation.

Scientific Area:

Welcome session / **22**

Presentation C2TN

Scientific Area:

Materials and technologies for Health and Environment (Posters) / **27**

Novel competitive binding membranes for the artificial kidney: towards enhanced removal Protein Bound Uremic Toxins

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Chronic kidney disease (CKD) has a prevalence from 11 to 13% in the world's population and the main treatment to replicate some of the kidney's functions is hemodialysis (HD) [1]. One of the biggest challenges of HD is the removal of the protein bound uremic toxin's (PBUT's) which, in blood, bond to albumin forming very large structures which cannot cross the membranes which compose the hemodialyzer or artificial kidney.
PBUT's such as indoxyl Sulfate (IS) and p-cresyl sulfate (pCS) are known to cause cardiovascular complications by inducing inflammatory responses or by causing endothelial or other vascular dysfunctions [1]. Hence, several studies focus on improving the removal of these toxins. A clinical study [2] has shown that certain pharmaceutical drugs, such as ibuprofen (IBU) and furosemide, bind more strongly to albumin than specific PBUT's, and that, by injecting large amounts of ibuprofen into the blood circulation of patients prior to undergoing HD, the removal of IS and pCS was enhanced. However, long-term administration of such large quantities of these drugs is unsustainable for the patient's health.
The main objective of this work is twofold: 1) to develop cellulose acetate (CA)/SiO2/(CH2)3NH2 monophasic hybrid membranes by coupling phase inversion and sol-gel technology [3] and functionalize them with IBU rendering (CA)/SiO2/(CH2)3NH2/IBU membranes; and 2) characterize them in terms of permeation performance. Control membranes were synthesized with methyl red dye (MR) in the location which will be occupied by IBU to have visual proof that the IBU molecules will be covalently bound to the polymer matrix. Results show that the (CA)/SiO2/(CH2)3NH2/MR monophasic hybrid membranes maintained the orange color after being stored for 40 days in deionized water. Dionized water permeation studies performed at flowrates between 30 and 130 mL/min and transmembrane pressures between 15 and 40 mmHg revealed that the hydraulic permeability of (CA)/SiO2/(CH2)3NH2/MR membranes is 49,1 mL/h.m2.mmHg and no dye was detected in the permeate nor the feed solution.

Materials and technologies for Health and Environment (Posters) / 28

Anti-fouling high flux ultrafiltration monophasic hybrid membranes for water treatment

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Titanium dioxide (TiO2) is currently one of the most common photosensitive materials used in photocatalysis due to its exceptional properties such as low cost, lower toxicity and high chemical content stability, being very useful in water treatment when combined with other components such as cellulose acetate (CA) [1].
Several integrally skinned asymmetric monophasic hybrid CA-based membranes were synthesized by coupling phase inversion and sol-gel techniques. Two series of membranes were synthesized: cellulose acetate/silica (SiO2)/Titania (95/3/2), CA/SiO2/TiO2 (90/6/4), CA/SiO2/TiO2 (85/9/6) and CA/SiO2 (95/5) in the first series; and CA/TiO2 (97/3) and CA (100) in the second series.
Hydraulic permeability (Lp) was studied, and the antibacterial properties of the membranes against Staphylococcus aureus, Escherichia coli, Enterococcus faecalis, Pseudomonas aeruginosa and Bacillus subtilis were evaluated with and without UV treatment, through 3 tests, changing only the way in which the active layer of the membranes was in contact with the bacteria.
The hydraulic permeability values were 12, 33, 7, 33, 27, 12 kg/m2.bar, for the membranes CA, CA/SiO2, CA/SiO2/TiO2 (95/3/2), CA/TiO2, CA/SiO2/TiO2 (90/6/4), CA/SiO2/TiO2 (85/9/6), respectively. In series 1, the addition of TiO2 to the membrane structure did not increase the Lp of the CA/SiO2/TiO2 membranes in relation to the reference membrane CA/SiO2, whereas for the CA/SiO2/TiO2 (95/3/2) membrane, Lp decreased with the addition of TiO2. In series 2, TiO2 increased the Lp of the CA/TiO2 membrane compared to the pure CA reference membrane.
In terms of antibacterial properties results revealed that all types of bacteria grow when placed in contact with the bottom porous layer of the membranes. When Bacillus subtilis was spread on top of the top active layer of the UV-treated CA/SiO2/TiO2 (95/3/2) membrane the bacteria created a "mucus", known to be produced as a form of resistance to activation. Further tests performed on

the CA/SiO2/TiO2 (90/6/4) and CA/SiO2/TiO2 (85/9/6) membranes showed that increase in the TiO2 content did not result in death of the bacteria.

Advanced materials and processes for Energy / **29**

Gamma irradiation as an alternative pre-treatment of macroalgae biomass for biogas production

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The anaerobic digestion of macroalgae is known for being a possible process to obtain biogas. However, due to the high organization of the macroalgae molecular structure, a pre-treatment is usually needed to improve the biogas production. In this context, gamma irradiation can be used as an alternative pre-treatment aiming to improve the digestibility of polysaccharides and other carbohydrates available in biomass and thus improve the biochemical conversion of biomass to biofuel.
To evaluate the efficiency of gamma irradiation pre-treatment, two algae, Saccharina latissima (SL) and Gracilaria gracilis (G) were selected. After preliminary studies, a dose of 20 kGy was applied to the dried algae using a dose rate of 0.7 kGy.h-1. Biogas was then produced through anaerobic digestion using as substrate synthetic food waste, and macroalgae as co-promoter of the digestion. Anaerobic digestate from wastewater sludge was used as inoculum.
Several analyses were carried out for the characterization of algae. Cumulative biogas production as well as the composition of the biogas was also studied as function of the different variables (algae SL/G), ratio substrate/algae, irradiated/non-irradiated algae).
Results indicate that irradiated macroalgae lead to higher biogas production yields in both studied algae.

Scientific Area:

Advanced materials and processes for Energy / **30**

Advanced Materials for Energy @ CF-UM-UP

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Energy considerations are essential in nowadays society and increasingly dependent on mobility and interconnectivity with the need to reduce the environmental impacts related to fossil fuels. The Centre of Physics at the University of Minho is undergoing competitive research in advanced materials for energy. Senen Lanceros is very active in the field of high energy density batteries, consisting in lithium-ion intercalation electrodes with a separator / electrolyte between them, to allow ionic conduction. Transparent thermoelectric thin films for thermal energy harvesting applications are being developed in the group of Carlos Envisaged applications are for hybrid photovoltaic systems and touch screens. The group of Bernardo Almeida researches in perovskite based nanostructured

multiferroic insulator oxide materials. The control of the electric and magnetic ferroic orders and their low joule heat dissipation offers pathways for multifunctional low power energy-efficient electronics. By using the electrospinning nanofabrication technique, Etelvina Gomes and co-workers produce novel piezoelectric nanofibers consisting of 3-nitroaniline nanocrystals embedded in PCL polymer. When subjected to a periodically applied force of 3 N, nanofibers generate a piezoelectric output voltage of 7 V, or 122 nWcm-2 power density. José Silva produces thermoelectric generators (TEG) and self-powered photodetectors based on ZnO and SnOx. In the case of the photodetectors, by combining a ZnO pyroelectric film with n-Si/p-SnOx heterojunction into one single structure, self-powered photodetectors based on the pyro-phototronic effect have been developed that demonstrate state-of-the-art performance. The 2D Materials and Devices group from Pedro Alpuim develops innovative techniques to produce 2D materials in the liquid phase over a large scale. Techniques such as liquid-phase exfoliation and shear mixing are studied and integrated to prepare different 2D Materials dispersions.

Scientific Area:

New principles and technologies for sensing / 31

Nanostructured plasmonic thin films for LSPR sensing applications

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Localized Surface Plasmon Resonance (LSPR) phenomenon in materials with noble metal nanoparticles is a hot topic due to the unique optical properties of the nanoparticles. Their optical response can be tailored by changing the size, shape and distribution, as well as the refractive index of the surrounding dielectric matrix [1,2]. If the nanoparticles are embedded in a porous host matrix produced using a GLancing Angle Deposition (GLAD) system, analyte molecules should easily diffuse to the vicinity of the nanoparticles and induce subtle changes in the refractive index. These interactions can be detected by monitoring the shape of the LSPR band in transmittance mode (T-LSPR) [3,4] and, therefore, several transduction mechanisms can be used to build T-LSPR sensors.
This work combines (i) the preparation of nanostructured plasmonic thin films using the GLAD system, up to incidence angles of 85º, (ii) sensitivity studies using High-Resolution LSPR Spectroscopy and (iii) LSPR band processing. Refractive index sensitivity studies were conducted in a controlled atmosphere chamber with real-time T-LSPR monitoring. The obtained signals were then processed using an algorithm that analyses changes in several parameters of the LSPR band. The results showed that the films deposited with a higher GLAD angle manifest enhanced sensitivity to gaseous atmospheres, thus confirming the possibility of using these nanostructured plasmonic thin films as T-LSPR sensors.

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Scientific Area:

New principles and technologies for sensing / 32

All-Printed Smart Label with Integrated Humidity Sensors, Communication System and Power Supply

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Sensing smart labels are an essential component of the Internet of Things (IoT) paradigm to provide the necessary information and data. The emergence of printing technologies applied to the field of materials, enables low-cost, flexible, easy-to-integrate sensors with tailored response [1, 2]. The combination of printing techniques along with new materials with tailored electrical and magnetic properties results in printed electronics, allowing a new generation of smart sensors, radio-frequency identification (RFID), photodetectors devices, transistors, and batteries.
Smart labels obtained by printing techniques are suitable solutions for low-cost devices with integrated electronic circuit for information processing, able to be incorporated in a variety of substrates, including flexible ones, for object recognition and tracking, composed by different sensors, including, temperature, pressure, or humidity. Still, the widespread use of these labels into functional devices requires easy integration and power supply. In this work[3] a smart label was developed with integrated humidity sensor and printed battery. The smart label is composed by detection, communication, control, and energy subsystems. It is based on a screen printed RLC circuit and a printed humidity sensor with electrical linear response. The printed battery based on lithium iron phosphate as an active cathode material is fabricated with six single cells connected in series, leading to ≈100 mAh g-1. The printed humidity sensor shows a linear response with relative humidity (RH) variation sensitivity of 0.004/%. Thus, it is demonstrated the development of fully printed smart labels, improving integration into a variety of applications.

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Scientific Area:

New principles and technologies for sensing

Advanced Materials and Processes for Energy (Posters) / 33

Study of transparent Thermoelectric ZnO-based Thin Films for Energy Harvesting through Atom Probe Tomography

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The design of a transparent thermoelectric material is a promising technology for touch–screen displays and solar cell applications, rendering a more sustainable powering of the device. In order to enhance the thermoelectric performance, the films must have a high Seebeck coefficient, high electrical but low thermal conductivity [1]. For this purpose, ZnO thin films were deposited by magnetron sputtering, and doped with Ga or Al and Bi. The approach consists in introducing Bi ions, a higher mass element, into the ZnO metal-oxide matrix, in order to hinder phonon mediated heat conduction, consequently reducing the thermal conductivity [2]. This work focuses on the Bi doping effect on ZnO, ZnO:Ga and ZnO:Al thin films. From Atom Probe Tomography (APT) analysis we determine the composition and investigate the cation and anion segregations to interfaces and grain boundaries. Based on thermal conductivity results obtained by Frequency Domain Thermoreflectance it is concluded that the doping of ZnO films with Al or Ga has a significant effect on thermal conductivity in contrast to the doping with Bi. This result can be understood by the fact that the Bi, unlike Al and Ga, is segregated at grain boundaries and does not substitute Zn in the crystal lattice. This last claim is unequivocally demonstrated by measurement results of APT and Transmission Electron Microscopy.

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Materials and technologies for Health and Environment (Posters) / 34

Magnetoliposomes Based on Shape Anisotropic Calcium/Magnesium Ferrite Nanoparticles as Nanocarriers for Doxorubicin

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The combination of liposomes with superparamagnetic nanoparticles allies the advantages of the widely used liposomal systems and the possibility to magnetically guide, selectively accumulate, and control the release of drugs on target. The effectiveness of the resulting structures –magnetoliposomes –is intrinsically related to the individual characteristics of the lipid formulation, the magnetic nanoparticles and their physicochemical combination. Herein, shape-anisotropic calcium-substituted magnesium ferrite nanoparticles (Ca0.25Mg0.75Fe2O4) were prepared for the first time, improving the magnetic properties of spherical counterparts [1]. The nanoparticles revealed a superparamagnetic behavior, high saturation magnetization (50.07 emu/g at 300 K), and a large heating capacity. Furthermore, a new method for the synthesis of solid magnetoliposomes (SMLs) was developed to enhance their magnetic response [1]. The manufacturing technicalities were optimized with different lipid compositions originating nanosystems with optimal sizes for biomedical applications (around or below 150 nm) and low polydispersity index. The high encapsulation efficiency of doxorubicin in these magnetoliposomes was proven, as well as the ability of the drug-loaded nanosystems to interact with cell membrane models and release DOX by fusion. SMLs revealed to reduce doxorubicin interaction with human serum albumin, contributing to a prolonged bioavailability of the drug upon systemic administration. Finally, the drug release kinetic assays revealed a preferable DOX release at hyperthermia temperatures (42 ºC) and acidic conditions (pH = 5.5), indicating them as promising controlled release nanocarriers by either internal (pH) and external (alternating magnetic field) stimuli in cancer therapy.

Materials and technologies for Health and Environment / 35

Production of Prebiotics from Pulp and Paper Industry Biomass

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During a pandemic when a healthy immune system is more significant than ever, prebiotics gain extra importance. These non-digestible food ingredients that stimulate the growth and/or function of beneficial intestinal microorganisms, protect against cancer and prevent cardiovascular and metabolic issues, are also known to play an important role in the improvement of the immune system [1].
In this work, a synergy is established between prebiotics increasing demand and pulp and paper industry, as xylooligosaccharides (XOS), emerging prebiotics obtained from xylan, are produced using bleached kraft pulp from Eucalyptus globulus from The Navigator Company.
Two different approaches for producing these prebiotics are studied and compared: enzymatic and acid hydrolysis. Higher yields of XOS, lower degrees of polymerization (strongest prebiotic activity [2]) and less production of unwanted by-products are obtained for the enzymatic approach. Additionally, the softer operating conditions and greener character of this process makes it the most promising choice for XOS production.
In conclusion, the production of these high-value products from this hardly explored raw material represents an excellent alternative for the pulp and paper industry to diversify/ innovate the pulp use and improve its competitiveness, also with excellent repercussions on the food and pharmaceutical industry.

Scientific Area:

Materials and technologies for Health and Environment (Posters) / 36

Study of waterproofing membranes used in civil construction to prevent corrosion induced by carbonation

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Reinforced concrete can suffer a significant reduction in durability when used under unfavorable exposure conditions. One of the main degradation mechanisms is corrosion induced by carbonation. This phenomenon occurs when atmospheric carbon dioxide penetrates the porous structure of concrete. Due to the alkaline nature of concrete, the steel covered by this material is protected from corrosion, since in this environment a film develops on the surface of the reinforced concrete, which consists of a layer of oxides with a protective function –a process referred to as passivation. When CO2 penetrates the porous structure of the concrete, it reacts with the calcium hydroxide leading to a decrease in pH, and as a result, the corrosion of steel commences. The need to develop efficient protection systems against carbonation by creating surface films that try to prevent the penetration of CO2 is in high demand.
The present work addresses the characterization of dense acrylic-based liquid membranes produced

at COLALIZ, Lda. in terms of CO2 permeability.
Three different flat sheet dense membranes consisting of three layers were prepared using dope solutions provided by COLALIZ, Lda using a 250 μm casting knife and were characterized in terms of surface morphology by scanning electron microscopy (SEM), chemical composition by attenuated total reflection - fourier transform infrared (ATR-FTIR) spectroscopy as well as CO2 permeability by the time-lag method. For comparison purposes, a certified waterproofing membrane used in civil construction that is already on the market was also studied.
Results show that the permeabilities of the COLALIZ membranes vary between 33 and 77 Barrer, where the membrane already on the market has a value of 33 Barrer.ATR-FTIR confirmed that these membranes are produced from styrene acrylic resins with main peaks appearing at 1560 cm-1 ,1780 cm-1, and 3020 cm-1, specific for styrene and acrylic groups respectively.

Quantum Materials and Quantum Technologies (Posters) / 37

Highly sensitive transparent piezoionic materials and their applicability as printable pressure sensors

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Hybrid materials based on ionic liquids (ILs) and polymers represent an emerging and interesting approach for an increasing number of applications, including sensors and actuators [1], as it represents a versatile way to produce particle free multifunctional materials with reduced environmental impact.
In this work, transparent piezoionic hybrid materials based on a thermoplastic elastomer styrene-ethylene-butylene-styrene (SEBS) containing 20 wt.% of the IL 1-butyl-3-methylimidazolium dicyanamide ([Bmim][N(CN)2]), suitable for pressure sensing applications, were prepared by the solvent casting method. The morphology, physico-chemical, electric, and electromechanical properties were evaluated.
The incorporation of [Bmim][N(CN)2] within the SEBS polymer matrix induced morphological variations with the presence of small voids within the polymer matrix. No significant physical-chemical changes occur upon the IL incorporation in the polymer, however an increase of the electrical conductivity from 1.44×10−14 Scm−1 to 2.94⊠10-11Scm-1 was observed. The piezoionic response was evaluated under loading and unloading compressive cycles with applied forces up to 5 N and 10 N, showing that independently of the applied force, the electrical resistance decreases with increasing pressure (Fig. 1a)). Additionally, a pressure sensitivity of approximately 25 kΩN−1 was observed, in a dynamic range from 0 to 10 N [2]
The suitability of the developed hybrid material as a transparent pressure sensor was evaluated through the development of a touch pad prototype compatible with printing technologies (Fig1b)).

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New principles and technologies for sensing / 38

Cylindrical Magnetic Nanowires for Information Storage Devices

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The urge for more efficient memory systems at low dimensions is a current requirement for the technological development of a wide range of applications, from industrial devices to daily life appliances. Among the possible candidates, cylindrical nanowires (NWs) have already shown their potential to increase storage density [1]; however, the device design still requires a magnetic tunnel junction as the writing component [2]. Recently we have proposed a new layout of multi-segmented magnetic NW arrays that could be used as 3D racetrack memory (RM) devices without the requirement of additional components [3]. The micromagnetic simulations revealed the feasibility of using a soft magnetic layer coupled to a hard magnetic segment as the writing section of the device (Fig. 1). Introducing additional in-line hard magnetic segments separated by non-magnetic chemical constraints would allow the creation of 3D RMs with enhanced efficiencies. However, no experimental evaluations have been performed so far.
This work provides the first experimental evidence of the fabrication of 3D RM devices with incorporated writing heads along the track. Using low-cost and high-yield template-assisted electrodeposition methods [4], single and multi-segmented NW hexagonal arrays (diameters of 50 nm and interwire distances of 100 nm) of NiCu and FeCo/Au were fabricated. A throughout magnetic characterization using hysteresis loops and first-order reversal curves (FORCs) revealed that the soft segment (NiCu) induced the reversal of the hard segment (FeCo) in a two-step process, reducing its coercive and effective anisotropy fields when coupled [5]. FORC diagrams also illustrated a fingerprint typically present in soft/hard magnetic interacting bi-layered NWs, confirming the strong interface coupling.
This work was developed under the framework of project POCI-01-0145-FEDER-028676.

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Scientific Area:

39

Luminescent poly(vinylidene fluoride)-based inks for anti-counterfeiting applications

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Counterfeiting is a high-tech crime that increasingly menaces governments, companies, and consumers. This ever-growing phenomenon affects severely national and international security, has a major detrimental impact on commercial and industrial activities and in some cases, may also put people's health and lives at risk [1]. Consequently, the development of anti-counterfeiting technological platforms is of fundamental importance in order to protect people from fraud and physical harm (in the case of pharmaceuticals).
The present work focus on the development of a new photoluminescent security ink composed of poly(vinylidene fluoride) (PVDF) [2] and the ionic liquid (IL) 1-butyl-3-methylimidazolium tetrakis(thenoyltrifluoroacetonato)eu ([Bmim][Eu(tta)4])[3]. The material exhibits high thermal stability up to approximately 267 °C, high chemical stability (inertness with respect to ethanol), high photostability and intense red emission when excited by long UV radiation (365 nm) with a maximum quantum yield value of 0.10±0.01 (Fig.1 a-b). As a proof of its applicability for authentication purposes, the security ink was screen-printed on a medical N95 protection mask, changing from transparent (under white light) to an intense red color emission under the irradiation of a commercial 365 nm LED as presented in Fig. 1c.

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Materials and technologies for Health and Environment (Posters) / 40

Micropatterned Electroactive Scaffolds for bone tissue engineering

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Bone tissue is naturally sensitive to mechano-electrical cues provided by its microenvironment. Tissue engineering relies on the development of scaffolds suitable to apply specific stimuli in order to recreate bone tissue microenvironments and trigger their natural recovery. The morphological clues of scaffolds can determine cell behavior and, therefore, the patterning of electroactive polymers can be a suitable approach for bone tissue engineering. This work reports on the influence of electroactive poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) micropatterned scaffolds in the adhesion, proliferation, and differentiation of bone cells. The micropatterned scaffolds were developed resorting to soft lithography in the form of arrays of lines, intermittent lines, hexagons, linear zigzags and curved zigzags with dimensions of 150 μm. Structures with more and less anisotropy –hexagons and lines, respectively –were selected to evaluate the influence of different sizes dimensions (25, 75, and 150 μm) in bone cells adhesion and proliferation. Differentiation tests were also performed on the intermediated size of 75 μm hexagons and lines patterns. The results shown that cell adhesion site and orientation of pre-osteoblasts can be controlled by the topography of the scaffolds [1]. Moreover, it is demonstrated that more anisotropic surface microstructures are able to promote bone differentiation without the need of further biochemical stimulation [2]. This work proves the relevance of patterned scaffolds to induce proper tissue regeneration.

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41

Electroactive materials for a new generation of antimicrobial surfaces

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Alternative antimicrobial approaches capable of avoiding resistance mechanisms in bacteria are extremely needed due to the alarming emergence of antimicrobial resistance. The application of physical methods in alternative to the common chemical ones represents an important breakthrough for such purpose [1].
In this study, electroactive nanocomposites composed of poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) and green-synthesized silver nanoparticles (AgNPs) were produced to prevent microorganisms'colonization. By applying a mechanical stimulus to the nanocomposite, which ultimately mimics movements such as walking or touching, an antimicrobial effect is obtained, resulting from the synergy between the electroactive microenvironments created on the surface of the material and the AgNPs. Both porous and non-porous PVDF-TrFe have shown antibacterial characteristics when stimulated at a mechanical frequency of 4Hz, being the effect boosted when AgNPs were incorporated in the films, reducing in more than 80 % the Staphylococcus epidermidis bacterial growth in planktonic and biofilm form. The electroactive environments sensitize the bacteria allowing the action of a low dose of AgNPs (1.69 % (w/w)). Significantly, the material did not influence the viability of mammalian cells, indicating that it is biocompatible. A piezoelectric stimulation of PVDF polymer films can provide an advance in antibacterial coatings for healthcare applications [2].

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New principles and technologies for sensing (Posters) / 42

Scalable wax-printing nanoimpregnation method for paper-based sensors and actuators

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Paper-based advanced functional materials have become the focus of intense research in recent years. Particularly, magnetic papers show strong potential for applications in a wide range of technologies including communication, magnetic sensing, electromagnetic filtering, magnetic-based health care tools, point-of-care microfluidic devices, and security, among others1,2.
In situ and lumen-loading, the main methods to prepare magnetoactive papers, show problems such as the rigorous reaction conditions, hard control of deposition location, decreased tensile strength, poor retention of magnetic nanoparticles, or the requirement to perform the magnetic impregnation during the papermaking process, that hinder their applicability3,4 . Those issues are addressed in the present work, in which ≈20 nm Fe3O4 nanoparticles are hydrothermally synthesized and later incorporated in a wax-based home-made cartridge and nanoimpregnated into paper by a thermal process leading to a magnetic paper with improved stress and strain at rupture and Young's modulus, 30 MPa, 4.5%, and 2 GPa, respectively, when compared to neat paper, 15 MPa, 3.5%, and ≈1 GPa, respectively. Additionally, the developed magnetic impregnation method provides the paper with a 0.2 emu g−1 magnetic saturation, allowing it to work as a bending actuator with a bending of 12 mm at an applied magnetic field of 105 mT. Such materials and optimized magnetic and mechanical features will enable applications in sensing, actuation, health care materials, or point-of-care devices, among others.

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43

All-printed magnetoelectric materials

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Two decades ago, the "polymer based magnetoelectric"idea changed thinking in magnetoelectric (ME) materials scientific community, which led to a new generation of high-performance materials and an increased focus on controlling structure, flexibility, and electrical output, as well as in the implementation into proof-of-concept applications1.
Nowadays, the successful implementation of those materials is closely related to the processing and integration of ME materials by additive manufacturing techniques 2.
Here a novel screen printed (Figure 1a), and flexible ME material is developed based on poly (vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) as the piezoelectric phase and poly (vinylidene fluoride) (PVDF)/CoFe2O4 as the magnetostrictive phase. The all-printed ME composite exhibits a

ferromagnetic behavior with ≈16 emu. g-1 saturation magnetization, ≈ -26 pC. N-1 piezoelectric response and a ME voltage coefficient (α) of ≈160 mV.cm-1. Oe-1 at the resonance frequency of ≈ 16 kHz (Figure 1b)3. Such optimized magnetic, piezoelectric and ME behavior associated to the reduced cost of assembly, easy integration into devices and the possibility to be obtained over flexible and large areas trough screen printing demonstrates the suitability of the developed material for applications in areas such as printed electronics, sensors, actuators, and energy harvesters.

Materials and technologies for Health and Environment (Posters) / **44**

Toluene removal from air based on sustainable membranes

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Outdoor and indoor pollutants have been identified as the main cause for the rising deaths by cardiovascular and respiratory diseases, with around 3.3 million deaths per year related to low air quality and with 98% of the low to medium income cities over 100000 habitants failing to meet air quality standards according to the World Health Organization. [1]
Among these pollutants, volatile organic compounds (VOC's) like toluene have been subject of attention in the last years due to its ubiquitous presence in car and wall paints, private homes, personal care products, and other man-made sources, being considered as one of the main contributors to smog, ozone layer depletion and global warming [2, 3].
Mitigation of this problem is being led by High-Efficiency Particulate Air filters (HEPA), active carbon filters, ionic generators and ultraviolet purifiers.
In this work, porous polymeric membranes based in natural polymers, such as alginate and carrageenan, were synthesized via freeze-dry method under different processing conditions to optimize pore size and porosity. The physical-chemical properties of the produced membranes were evaluated to assess their suitability towards VOC's removal. Additionally, a metal-organic framework (MOF808) loaded with three different amino acids incorporated into these membranes, showed promising adsorption and/or degradation of the selected VOC, with adsorption/degradation tests being performed, leading to a high efficiency removal (around 70%).

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Scientific Area:

Advanced materials and processes for Energy / **45**

OER/ORR bifunctional electrocatalysts based on PtM (M=Ni,Fe,Cu) supported on graphene nanoplatelets

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Three different Pt-M (M = Ni,Fe,Cu) based electrocatalysts were synthetised via simultaneous supercritical carbon dioxide (scCO2) deposition technique of nanoparticles on graphene nanoplatelets (GNPs). These were tested as electrocatalysts for oxygen reduction (ORR) and oxygen evolution (OER) reaction in metal-air batteries and unitized regenerative fuel cells (URFCs). Primary metal (Pt) and secondary metal (Ni, Fe, Cu) were deposited onto GNPs by scCO2 in the same step which resulted in ca. 20 wt.% Pt loading and M loading in the 1.4 - 3.4 wt.% range. Adsorption isotherms of the precursors onto the GNPs were used to determine desired amount of the corresponding precursors [1].
Linear scan voltammetry (LSV) experiments at different rotation rates were performed in alkaline medium (0.1 M KOH) in order to assess the electrocatalytic activity toward ORR and OER. Catalyst with Fe as secondary metal showed the highest diffusion-limited current density, jd, of -4.65 mA cm-2, followed by PtCu/GNPs (-4.37 mA cm-2) and PtNi/GNPs (-3.65 mA cm-2). It is worth noting that commercial Pt/C (40 wt.% Pt) catalyst tested in our previous work reached a jd value of -6.44 mA cm-2, comparable with herein tested catalysts [2]. PtFe/GNPs sample also showed the lowest value of Tafel slope (81 and 66 mV dec-1) and number of exchanged electrons value as high as 3.66, indicating direct 4e- O2 reduction to water. OER investigation revealed that catalyst with Fe as secondary metal also showed superior performance for this reaction as evidenced by the lowest OER onset potential, the highest achieved current densities, and the lowest value of Tafel slope. Moreover, ΔE, the difference between the potential at which OER achieves 10 mA cm-2 current density and half-wave potential of ORR, E1/2, has the lowest value for PtFe/GNPs sample (≈0.89 V). Thus it can be concluded that PtFe/GNPs catalyst exhibits promising ORR/OER performance. Further investigations will be focused on testing its long-term stability and performance in fully assembled URFC or metal-air battery.

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Advanced materials and processes for Energy / **46**

Enhancing the efficiency of alkaline water electrolysis by using ionic liquids as electrolyte additives

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Alkaline water electrolysis offers a possibility of producing hydrogen gas without consuming fossil fuels. Namely, the use of electricity from renewable energy sources makes the electrolysis process green and hydrogen gas a green energy carrier, enabling switching from carbon-based to green and sustainable energy sources. However, most of the global hydrogen is currently still produce by the steam reforming of fossil fuels [1]. Thus, increasing the efficiency of hydrogen and oxygen evolution reactions (HER and OER) is vital to make electrolysis economically viable and competitive to steam reforming. Research to improve the efficiency of the electrode reactions is mainly focused on developing novel electrocatalytic materials. Another approach to decrease the electrode reactions activation overpotential is use of electrolyte additives, such as room temperature ionic liquids (RTILs). RTILs can be tailor-made to increase their beneficial effect on the HER and OER kinetics. Improved HER kinetics in the presence of RTILs has been previously confirmed in both acidic and alkaline media [2,3]. The present work examines four new tailored RTILs having the same chloride anion, and methylimidazolium cation containing different alkyl chains. These include 3-ethyl-1-methylimidazolium chloride, 3-butyl-1-methylimidazolium chloride, 3-(2-methoxyethyl)-1-methylimidazolium chloride, and 3-(2-ethoxyethyl)-1-methylimidazolium chloride. The effect of the addition of small amounts (1 vol.%) of the listed RTILs on HER and OER kinetics in alkaline media (8 M KOH) is assessed using Pt electrodes. Cyclic voltammetry, linear scan voltammetry, and chronoamperometry are carried out at temperatures ranging from 25 °C to 80 °C. Evaluation of kinetic parameters was carried out and their values were compared with previously reported data. Finally, measurements of the volume of generated gas were done in a small-scale alkaline electrolyser to compare the gas production in pure 8 M KOH solution and after the addition of the chosen RTILs.

Materials and technologies for Health and Environment / **47**

Out-of-field doses in radiotherapy treatments of paediatric patients

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Out-of-field doses are delivery to healthy tissues, which may allow the development of second tumours. Its evaluation with MC methods is essential since these doses are inaccurate when calculated by TPSs. The use of IMRT has been discussed, especially in paediatric patients, as it leads to a “bath” of low doses to large volumes of out-of-field tissue.
This study aims to evaluate out-of-field doses in paediatric tumours by comparing 3DCRT and IMRT techniques. Thus, a computer model of a LINAC, as well as its 6 MV energy photon beam, and MLC, were initially modelled and validated in MCNP6. Subsequently, CT images of a paediatric anthropomorphic phantom were acquired in IPOLFG and with the ImageJ program; a voxelized paediatric computational phantom was created. Two dosimetric plans were performed, one with the 3DCRT technique and the other with the IMRT technique.
Experimental measurements were carried out in LINAC with the paediatric anthropomorphic phantom and with TLDs reproducing the treatment plans previously created in TPS.
In the MCNP6 program, the model of the LINAC was added in an unprecedented way, with its MLC and the 6 MV energy photon beam, as well as the previously created voxelized phantom and the out-of-field doses for all organs were calculated for both techniques.
The results have shown that out-of-field doses can be seriously underestimated with TPSs. The out-of-field doses are higher when using the IMRT technique (right eye = 13040.6 mGy), compared to the 3DCRT technique (right eye = 593 mGy).
This study demonstrates a powerful combination of (1) dosimetric measurements in a clinical environment, (2) modelling of a LINAC, treatment beam and MLC, (3) out-of-field organ doses in a paediatric phantom, (4) creation of a voxelized paediatric phantom. This could have an impact in radiological protection and dosimetry in radiotherapy services.

Advanced Materials and Processes for Energy (Posters) / 48

Towards environmentally friendly solution-processed CIGS photovoltaic devices

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Strong efforts are being carried out looking for efficient, clean and renewable energy sources to meet the decarbonization goals. With respect to solar energy, thin film photovoltaic (PV) systems based on CuInxGa1-xSe2 (CIGS) deserve special attention, due to its outstanding opto-electronic properties. Despite the high-efficiency devices produced by vacuum deposition processes, non-vacuum ones are desirable due to the lower cost of the process, scalability, and compatibility with large areas and flexible substrates. To date, solution-processed CIGS thin film solar cells with an efficiency of 17.3% [1] have been achieved, however highly toxic solvents are used.

To this end, a water-based ink comprising well-dispersed Cu, In and Ga oxides was screen-printed into fluorine tin oxide (FTO)-coated soda-lime glass (SLG). After deposition, selenization was used to convert the oxides into CIGS crystal and the resulting thin films show homogenous thickness of ≈2.5 μm and nominal Cu0.92(In0.77Ga0.31)Se2 composition. To complete the PV device, a buffer layer of CdS was deposited by chemical bath and the i-ZnO/ZnO:Al top conductive layers were sputtered. The resulting device revealed a record-breaking for screen printed CIGS photoabsorbers with 7.9% of efficiency (Figure 1a). Moreover, all-solution-processed CIGS PV cells with the same photoabsorber and CdS layers, and spray-coated water-based inks of i-ZnO/indium tin oxide (ITO) as top conductive layers were fabricated, demonstrating an efficiency of 2.2% (Figure 1b).

This abstract is being submitted for a poster presentation.

Materials and technologies for Health and Environment (Posters) / 49

New generation of ionic liquid-based materials for tissue regeneration applications

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As the main goal of tissue engineering (TE) is to mimic cellular microenvironments through scaffold systems, there has been growing interest in smart and functional materials, namely electroactive ones, to develop active scaffolds for TE applications since they are able to provide, apart from the structural support, the necessary biochemical and biophysical cues to cells in order to promote their growth and differentiation [1]. Currently, TE is taking advantage of ionic liquids (ILs) to

develop ionic polymer-based materials with tailored piezo-ionic conductivity, suitable for muscle tissue regeneration [1,2]. Their unique properties, such as high electrochemical and thermal stability, high ionic conductivity and low vapor pressure, make ILs highly attractive for TE applications [1,2]. This work reports on the development and application of ionic electroactive materials based on piezoelectric polymers and ILs for TE. For that, biocompatible piezoeletric polymers such as poly(vinylidene fluoride) (PVDF) and its copolymer, poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE), were combined with different ILs, (choline dihydrogen phosphate ([Ch][DHP]), choline bis(trifluoromethylsulfonyl)imide ([Ch][TFSI]) and choline acetate ([Chol][Ac]), and processed in the form of films by solvent casting and fibers by electrospinning up to a maximum of 20% wt. of IL content. Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) was used as well as a polymer matrix aiming to develop ionic polymer-based materials which are biocompatible and biodegradable. The morphological, physico-chemical and thermal properties of the composites were evaluated, as well as their potential use as scaffolds for TE applications. Results demonstrated that the incorporation of IL into the polymer matrix influences the microstructure, wettability, surface topography as well the thermal stability of the composites. Moreover, it was verified that, in some cases, IL incorporation affects the crystallization process of the polymer, acting as a defect during its crystallization. The noncytotoxicity of the developed ionic polymer-based materials indicates their suitability for TE applications.

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Materials and technologies for Health and Environment (Posters) / 50

Tridimensional cellular models of prostate cancer for the evaluation of copper-64 chloride as a theranostic agent

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Prostate cancer (PCa) is one of the most common cancer types in men, and, despite the advances that led to a decline in mortality, it is still considered incurable in advance stages. Thus, it is exceedingly important to ensure an early diagnosis and develop new approaches to overcome PCa chemoresistance. Radiopharmaceuticals emerge as possible solutions for this challenge, as they have the potential to be used in diagnosis, therapy or even simultaneously for both purposes (theranostics). In particular for PCa, it was already demonstrated by the Radiopharmaceutical Sciences group that copper-64 chloride (64CuCl2) has the potential to induce damage in monolayer cultured PCa cell lines, while bearing minimal side effects in non-tumoral cells, being a promising theranostic agent for PCa [1]. Nevertheless, the monolayer culture model has a limited predictive value, and results obtained might not be translatable in vivo. Multicellular tumor spheroids are a 3D culture model that overcome some of the limitations of the monolayer model, replicating the metabolic and proliferative gradients of in vivo solid tumors. Furthermore, unlike the monolayer model, the spheroids have an increased population of cancer stem cells (CSCs), involved in increased tumor resistance and recurrence [2].
In this work, we further assessed the theranostic potential of 64CuCl2 using PCa spheroids to better replicate the in vivo tumor environment [3]. After the initial establishment and characterization of the morphology and CSCs populations of spheroids derived from three PCa cell lines (22RV1, DU145 and LNCaP), we assessed the cellular uptake of 64CuCl2. We also evaluated changes in the growth profile and viability of the spheroids exposed to 64CuCl2, along with the clonogenic capacity of spheroid-derived cells. The results obtained revealed that 64CuCl2 is able to significantly reduce the spheroids' growth and viability, as well as their reproductive capacity. Interestingly, the spheroids with the highest initial percentage of stem-like cells, derived from the DU145 cell line, were found to be the most resistant to 64CuCl2.

Materials and technologies for Health and Environment / 51

Multifunctional Gold Nanoparticles for Cancer Theranostics

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Radionuclide therapy is an anticancer therapeutic modality based on the use of radiopharmaceuticals, which are drugs containing radionuclides emitting ionizing radiation (β- and α particles or Auger-electrons). Many of these radionuclides are also gamma- or positron-emitters and then are suitable for imaging applications using single-photon emission computerized tomography (SPECT) or positron emission tomography (PET) imaging, respectively. This possibility renders some radiopharmaceuticals intrinsically suited to provide therapeutic effects and, simultaneously, to monitor non-invasively therapeutic outcome in real-time. Therefore, radionuclide therapy has unique advantages within a theranostic approach for cancer when compared with other therapies, showing a great promise towards the application of precision and personalized medicine. To fully profit from these advantages, it is essential to design "smart"radioconjugates (molecular or nanosized) that specifically recognize the target tumoral cells to enhance the therapeutic effect and spare the surrounding normal cells from radiation damage.
In this communication, we will present relevant contributions of the C2TN team in this field, focusing on gold nanoparticles (AuNPs) (Fig. 1) [1] targeted at the gastrin releasing peptide receptor (GRPr) overexpressed in several tumors, like prostate cancer and glioblastoma multiforme. The strategies used to design these molecular or nanosized GRPr-targeted conjugates will be summarized, as well as the different biological studies employed in their preclinical evaluation. It will be highlighted how a combination of expertise is required to elucidate the theranostic potential of these target-specific radioconjugates, spanning from radiopharmaceutical sciences (e.g., ligand design, labelling chemistry, metabolism and biodistribution studies) to radiobiology (e.g. assessment of DNA damage and cellular viability) and physics (e.g., micro-and nanodosimetric calculations at the cellular and the DNA level).

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Scientific Area:

Materials and technologies for Health and Environment (Posters) / 52

A Bioorthogonal Chemistry Approach for Peptide Receptor Radionuclide Therapy (PRRT)

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Pre-targeting approaches based on the inverse-electron-demand Diels-Alder (iEDDA) reaction between strained trans-cyclooctenes (TCO) and electron-deficient tetrazines (Tz) have emerged in recent years as valid alternatives to classic targeted strategies to improve the diagnostic and therapeutic properties of radioactive probes. As reported in this communication, we have synthesized a small family of clickable chelators and proceeded with their labeling with medically relevant radiometals (e.g. 111In, 177Lu and 90Y) to explore pre-targeting strategies, based on in vivo click chemistry [1]. In particular, the [90Y]Y-DOTA-Tz complex was evaluated in a prostate cancer PC3

xenograft by ex-vivo biodistribution studies and Cerenkov luminescence imaging (CLI). The studies comprised the injection of a clickable bombesin (BBN) antagonist in the tumour-bearing mice followed by the radiocomplex [90Y]Y-DOTA-Tz, and the mice imaged by CLI at different post-injection times (p.i.). Analysis of the images 15 min and 1 h p.i. pointed out an encouraging quick tumour uptake with a fast washout, providing a preliminary proof of concept of the usefulness of the designed clickable complexes for pre-targeting strategies. To the best of our knowledge, the use of peptide antagonists for this purpose was not explored before. However, further investigations are needed to optimize the pre-targeting approach based on this type of biomolecules and evaluate its eventual advantages.

[1] Alice D'Onofrio et al., Frontiers in Medicine 8, 647379 (2021).

Advanced Materials and Processes for Energy (Posters) / **53**

Self-assembly of bis-salphen metal-organic frameworks: atomistic perspective

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The recently-observed[1] self-assembly of salphen-based metal-organic frameworks (MOF) into networks of interconnected microrings with nano-thin strings may suggests a new intriguing tool for nanoscale patterning. In particular, their ability to align very small amounts of carbon nanotubes into ultra-low density percolating network promises a breakthrough in creating highly transparent flexible thin film electrodes for illumination panels and light harvesting devices.
However, the mechanism of this phenomenon yet needs to be clarified. In this work we will show how atomistic simulations help to shed light on supramolecular structure and details of the formation of this unusual self-assembly pattern.
We use ab initio calculations and all atomic molecular dynamics simulations in explicit together with umbrella sampling and free energy perturbation to investigate conformational space of the bis-salphen MOFs and potential self-assembly pathways.
We observe that a particular conformation of the bis-salphen MOF allows it to form dimeric units, capable of linking with other units via either pi-pi or coordination Zn-O interactions in the two orthogonal directions. Due to these interactions bis-salphen MOFs can self-assemble into supramolecular chains, sheets and tubes, with highly variable mechanical properties. Furthermore, we show that the free energy gains of the two self-assembly pathways are determined by the solvent, which allows to control geometry of self-assembly and helps to relate our predictions to experimentally observed patterns.
We propose[2] that the compounds under study form a 1D coordination polymer, the fibres of which are elastic enough to fold into toroidal globules upon solvent evaporation, while being able to link separate chains into extended networks. We also explain the separate roles of atomic groups, constituting the molecule and the way solvent controls the self-assembling structure.
Intended for poster presentation.

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New principles and technologies for sensing / **54**

Gas sensor based on Au nanoparticles embedded in a CuO matrix by HR-LSPR spectroscopy at room temperature

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Gas sensing, based on bulk refractive index (RI) changes, has been a challenging task for localized surface plasmon resonance (LSPR) spectroscopy [1]. In this work, it is demonstrated that a plasmonic thin film composed of Au nanoparticles embedded in a CuO matrix can be used to detect small changes (as low as 6×10-5 RIU) in bulk RI of gases at room temperature, using a High-Resolution LSPR spectroscopy system [2,3]. Such thin film system was optimized by reactive magnetron sputtering, followed by an in-air annealing protocol treatment at 700 ºC to promote the Au nanoparticles growth. To enhance the film's surface activity, a simple Ar plasma treatment revealed to be enough to remove the top monolayers of the film and to partially expose the embedded nanoparticles, and thus promoting the film's gas sensing. The treated sample exhibit high sensitivity to inert gases (Ar, N2), presenting a refractive index sensitivity to bulk RI changes of 425 nm/RIU. Furthermore, a 2-fold signal increase was observed for O2 and CO gases, showing that the thin film system is clearly more sensitive to these non-inert gases, due to, most probably, gas adsorption on the film surface. The results show that the Au:CuO thin film system has a high sensitivity to detect small RI changes caused by different gases, supporting the potential of this thin film system to be employed as a gas sensor, particularly in CO detection.

Scientific Area:

New principles and technologies for sensing

Materials and technologies for Health and Environment (Posters) / 55

Organelle-Targeted Radioconjugates for Cancer Theranostics

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The radiobiological effects induced by Auger electron (AE) emitters might include hardly repairable and severe DNA damage in the targeted tumor cells, if the AEs are emitted in close proximity to a radiosensitive cellular target, such as the nuclear DNA or the mitochondria. Towards this goal, we have designed organelle-targeted 99mTc-complexes with the ability to selectively recognize prostate cancer cells, using 99mTc as a readily available model radionuclide to validate the design of new classes of AE emitting radioconjugates for targeted radionuclide therapy (TRT) of cancer. The designed compounds include dual-targeted complexes carrying a bombesin (BBN) peptide recognizing the gastrin releasing peptide receptor (GRPr) and an acridine orange (AO) or a triphenylphosphonium (TPP) group. The GRPr is overexpressed in a variety of cancers, namely prostate cancer (PCa). The AO group is a well-known DNA intercalator and the TPP group has well-recognized mitotropic properties. Thus, we have anticipated that the presence of these groups should enhance, respectively, the accumulation of the 99mTc radionuclide in the nucleus or mitochondria of the targeted PCa cells (Fig. 1). In this communication, we will report on the cellular internalization and subcellular localization of each type of dual-targeted radioconjugates, as well as on the study of their radiobiological effects in PC3 human PCa cells. In particular, this included the study of the influence of the different 99mTc-complexes in: i) the cellular proliferation rate; ii) the induction of DNA damage; iii) the mitochondrial function. The results obtained have since encouraged the application of this dual-target

approach to other AE emitters more suitable for Auger therapy of cancer, such as 111In and 161Tb, as explored by us within a recently approved FCT-funded project.

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New principles and technologies for sensing (Posters) / 56

Environmentally friendly, biocompatible graphene-based inks for all-printed temperature, deformation, and touch sensors

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The demand for advanced functionalities in electronic devices has been drawing growing attention in the scientific and industrial fields. Printed electronics present the advantages for low-cost and large-scale production, thus being subject of research in a wide range of applications across different sectors, including sensors, actuators, and electronic components. Graphene, a 2D material with exceptional mechanical, thermal, and electrical properties, represents an outstanding candidate for printed flexible electronics. Most graphene inks use organic solvents such as N-methyl-2-pyrrolidone and dimethylformamide, both being toxic, even at low concentrations, which precludes their use in industrial scale production. Therefore, there is an urgent need to replace those solvents by environmentally friendly ones.
In this work, a water formulation was developed with carboxymethyl cellulose, a natural polymer as a binder. The optimized formulation allowed a maximum electrical conductivity of ρ= 1.8×10-2 Ω.m in the conductive patters for printed electronics. The multifunctionality of the inks is demonstrated by being applied in thermosensitive [1], piezoresistive [1] and in an 8 inch touch sensor 2. A maximum thermoresistive sensitivity of S=-0.27, a piezoresistive Gauge-Factor of 1<GF<5 and a signal noise ratio of 10 demonstrate the suitability of the materials for temperature, deformation sensors and touch sensor applications, respectively. The multifunctionality of the materials is thus demonstrated as well as their potential for printed electronics while being both environmentally friendly and biocompatible.

Quantum Materials and Quantum Technologies / 57

Probing spin-waves in individual ferromagnetic nanoelements

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Materials and technologies for Health and Environment (Posters) / 58

Membrane-water partitioning to screen drug candidates: towards a high-throughput microfluidic platform

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In a rational drug design, the modulation of the chemical structure based on drug's pharmacokinetic profile can be the solution to improve drug development efficiency. Significant correlations between lipophilicity and membrane permeation have been established [1]. Further, anisotropic membrane-like systems, such as membranes/water (M/W) partitioning systems, are described as a more accurate alternative to octanol/water for the estimation of pharmacokinetic behavior [2]. In the present study, derivative spectroscopy was used to calculate M/W partition coefficient of two model drugs and to predict several parameters of their pharmacokinetic profile using lipid nanosystems of different constitution as biomembrane mimetic models (Fig. 1A) [3,4]. The obtained results highlight the relevance of using biomimetic models to determine the logM/W to obtain reliable information in the early stages of drug development. Notwithstanding, this methodology is being restricted mainly to the academic research. Their large-scale use at industrial level has been hindered mostly by its low throughput. The work presented here also considers the development of a microfluidic platform in which microchannels are coated with supported lipid bilayers that enable the assessment of the logM/W partitioning of drugs (Fig. 1B). This microfluidic platform constitutes a promising high-throughput technology to screen drug candidates at a large scale fulfilling the requirements from pharmaceutical and cosmetic industries.

Advanced Materials and Processes for Energy (Posters) / 59

Ferroelectric thin film nanostructures by laser ablation

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Multiferroic composite materials are of great interest for technological applications due to the magnetoelectric coupling effect, by which an electric (magnetic) field may be used to control the magnetization (polarization). Being insulators, these materials find application in low power energy efficient electronics, due to their low joule heating effect. In the form of thin films the magnetoelectric coupling can be considerably increased by strain engineering, by controlling the mechanical interaction and lattice mismatch across the substrate/film interface. Different deposition methods are available to produce the composite structures, with pulsed laser ablation in a background gas being noteworthy for its simplicity and precise control of the deposition parameters, namely the target-substrate distance. However, the optimization of the deposition parameters to obtain films with the desired microstructure is still performed on a trial and error basis, justifying the modelling of the ablation plume dynamics with the background gas in order to try and predict the resulting film structure.
In this study, multiferroic composite systems were produced by pulsed laser ablation. The systems studied consisted of lithium niobate ($LiNbO_3$, ferroelectric) thin films deposited on Si and Si\Pt substrates, and bi-layer $LiNbO_3$ \ $CoFe_2O_4$ (cobalt ferrite, ferromagnetic) thin films deposited on Si\Pt substrates. $LiNbO_3$ possesses high piezoelectric and electro-optic properties while $CoFe_2O_4$ has high magnetostriction, saturation magnetization, coercivity and magnetocrystalline anisotropy. The

films were deposited at 650 ºC and at room temperature, with the latter submitted to an annealing procedure post-deposition. Different combinations of pressure and target-substrate distance were used. The resulting films were studied using scanning electron microscopy and focused ion beam. The film thickness and grain size generally increased with deposition time.
The ablation plume dynamics in a background gas were modelled according to a blast wave model [1], providing an equation for the propagation of the shock front and allowing the determination of a pressure-distance relationship [2]. A phase diagram of the zones of Thornton's diagram [3] was built for both deposition temperatures, predicting the resulting zone structure for a given pressure and distance. The Thornton's zones observed in the samples indicate the existence of an optimal value of deposition parameters, striking a balance between film crystallinity and adequate microstructure, but without increasing the thickness to the extent of inhibiting surface diffusion or inducing structure relaxation in the films.

Scientific Area:

Materials and technologies for Health and Environment (Posters) / 60

Electrospun nanofibers loaded with Truvada® as a novel intravaginal delivery system for HIV prophylaxis

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HIV stands as an increasing global burden and sexual transmission remains the leading cause of new infections, particularly in women in the Sub-Saharan region [1]. New prevention strategies are urgent and vaginal microbicides have proven to be promising alternatives to prematurely fight and control its dissemination. In this study, we developed TDF/FTC-loaded fibers and tested their pharmacokinetics (PK) compared to oral Truvada® [2].
Hydrophobic and hydrophilic fibers were produced by electrospinning using polycaprolactone (PCL) and poly(vinyl alcohol) (PVA) with drug-loaded liposomes (DMPC:Chol:DOPE, 7:2:1), respectively. They were further characterized regarding their: (i) size and morphology; (ii) structure and mechanical properties; (iii) drug loading and in vitro drug release; (iv) interaction with mucin molecules; and (v) in vitro cytotoxicity using the MTT metabolic activity assay. Additionally, PK were assessed in medroxyprogesterone- treated ICR mice. Drug levels in vaginal lavages, vaginal tissues and blood plasma were determined by LC-MS/MS after vaginal administration of fibers (70 µg/50 µg of TDF/FTC) and compared to the continuous treatment with daily oral Truvada® (61.5 mg/mg per kg).
The mean section diameter of PCL and liposomes/PVA fibers was of ≈700 nm and ≈150 nm, respectively. Furthermore, the strong interactions observed with mucin molecules anticipate that all fibers may promote higher vaginal retention times. TDF/FTC release profiles were fast and almost all incorporated drug was released within 15-30 min in micellar medium (pH= 4.5). The toxicity of drug-loaded fibers to CaSki and HEC-1-A genital cell lines was negligible. In vivo experiments showed that liposomes/PVA fibers were able to significantly enhance the concentrations of TDF, tenofovir (TFV; resulting from TDF
®
hydrolysis) and FTC, as compared to PCL fibers and oral Truvada . Relative bioavailability
(Frel) values of TFV and FTC were 4.0 and 29.4, respectively, as compared to Truvada® (TDF was not detected for oral treatment). PCL fibers also featured higher drug levels in lavages than oral Truvada® (Frel values for TFV and FTC were 2.3 and 2.4, respectively).
Our results suggest that liposomes/PVA fibers may constitute an interesting system for the vaginal delivery of TDF/FTC in the context of topical pre-exposure prophylaxis.
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Advanced Materials and Processes for Energy (Posters) / 61

Integrated study of triboelectric nanogenerators for ocean wave energy harvesting: Assessing their behavior in model buoys and real sea conditions

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Ocean related activities are often supported by offshore equipment with particular power demands. These are usually deployed at remote locations and have limited space, thus small energy harvesting technologies, such as photovoltaic panels or wind turbines, are used to power their instruments. However, the inherent energy sources are intermittent and have lower density and predictability than an alternative source: wave energy [1]. The triboelectric nanogenerator (TENG) is a promising and efficient energy harvesting technology capable of addressing these problems as it can efficiently convert regular/irregular external mechanical energy into electrical power based on the triboelectrification and electrostatic induction effects [2-4]. In this work, three TENGs based on rolling-spheres were developed and their performance compared in both a "dry"bench testing system under rotating motions, and in a large-scale wave basin under realistic sea-states installed within a scaled navigation buoy. The experiments showed that the electrical outputs of these TENGs tend to rise with increasing pitch amplitudes and decreasing period due to the increase of the spheres'velocity. The capability of these TENGs to harvest energy from ocean waves when incorporated into a navigational buoy was demonstrated under realistic sea states. The voltage generated by the TENGs achieves maximum values for periods close to the natural period of the scaled buoy (˜ 0.92 s). The wave basin tests clearly demonstrated a significant dependency of the electrical outputs on the pitch degree of freedom and the need to consider the full dynamics of the buoy, and not only that of TENGs, when subjected to the excitations of waves.

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Advanced Materials and Processes for Energy (Posters) / 62

Enhancing the optical properties of black conventional colorants by TiO2 incorporation

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In Europe, buildings are responsible for over 40% of energy consumption and greenhouse gas emissions, so that improving their sustainability is a much-needed demand for the construction sector.

To reduce energy use and CO2 emissions, it is necessary to contain as much as possible the energy requirements of a building [1]. Among the several solutions studied, the development of materials with high reflectance of the solar energy for roofs and envelope systems has been shown to be effective in reducing the thermal gains and overheating in buildings [2]. A cool material is a material that contains highly near-infrared reflective pigments and that can be applied onto a surface exposed to solar radiation to reduce its radiation absorption. Thus, the use of coatings containing such reflective materials that reflects a large part of solar radiation is decisive to reduce the thermal gains and overheating of buildings [3]. Our study targeted the development of innovative envelope systems by increasing their solar reflectance through new material formulations with the inclusion of nanoparticles. For that, it is necessary to develop and optimize nanoparticles formulations to achieve a high NIR reflectance. We studied the reflectance and colour properties by doping a standard black coating with different sizes of TiO2 nanoparticles, in an acrylic substrate. In particular, titanium dioxide rutile nanoparticles were used with the concentration in the coating being varied (1%, 3%, 5% and 8%). The inclusion of the TiO2 nanoparticles in these coatings led to an increase in the spectral reflectance in the acrylic substrate, with the most promising results obtained for composites containing TiO2 with 30 nm and with 20% concentration (with a 0.23 reflection compared to 0.13 for the standard colorant). Our results indicate that, with increasing nanosized particles content, the thermal insulation properties for the coating are improved.

Advanced Materials and Processes for Energy (Posters) / **64**

Direct-Ink-Writing of Electroactive Polymers for Sensing and Energy Storage Applications

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The growing concerns on environmental impact require a new generation of materials and processes for sustainable electronics and energy storage systems [1]. In this scope, additive manufacturing techniques arise as an effective process to improve the sustainability of device fabrication [2]. In this work, direct-ink-writing was used to produce poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) films and membranes. Different parameters were variated such as solvent evaporation temperature and fill density percentage, which allowed to obtain different morphologies, including dense films and porous membranes. In addition, the different conditions allowed to tune electroactive ⍁-phase content, thermal and mechanical properties. The prepared PVDF-HFP films with a fill density of 80 and a solvent evaporation temperature of 50 ℃, show a dielectric constant of 16 at 1 kHz and a piezoelectric d33 coefficient of 4 pC.N-1. The porous structured samples were applied as separators for lithium-ion batteries. The highest ionic conductivity (3.8 mS.cm-1) is achieved for the sample with a fill density of 100 and a solvent evaporation temperature of 25 ºC. The assembled batteries present excellent cycling performance, achieving values up to 130 mAh.g-1 at C/8 rate. With this work, the versatility of the printing process is demonstrated, allowing the fabrication of advanced materials for high-end applications.

Advanced Materials and Processes for Energy (Posters) / **65**

Transparent piezoelectric polymer-based materials for energy harvesting and touch detection devices

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Energy harvesting devices allowing to recover wasted energy from the environment are increasingly developed. Mechanical energy is the most interesting sources of power for energy harvesting and piezoelectric materials present excellent overall properties for the scavenging of wasted energy. Piezoelectric polymers and, in particular, polyvinylidene fluoride (PVDF), show appropriate mechanical properties for large amplitude movements, higher piezoelectric coefficients, transparency, and be easily integrated into devices. A transparent piezoelectric energy harvesting device has been developed with screen printed transparent (72%) and conductive (42 Ω/sq) electrodes on PVDF sheets with a d33= -33 pC/N, generating about P˜12 μW and P˜8 μW under pressing and bending modes, corresponding to an energy per cycle of E˜ 37 nJ and E˜55 nJ, respectively. The piezoelectric energy harvesting characteristics of the materials was theoretical evaluated and the applicability of the materials for touch detection demonstrated.

66

Design and development of a third-harmonic generation setup for the characterization of the nonlinear optical properties of 2D materials

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Graphene - a single atomic layer of carbon atoms - is a very promising material, mainly due to its extremely high and broadband nonlinear optical susceptibility [1] and the possibility of occurrence of interband transitions at all optical frequencies. Ultrafast third-harmonic generation (THG) of ultrashort laser pulses in graphene allows not only the temporal characterization of the ultrashort pulses themselves but also the study of carrier dynamics in graphene. The possibility of obtaining an enhanced nonlinear signal when using multi-layer graphene [2] further adds to these capabilities. The technique of dispersion scan (d-scan) [3] developed in our group in collaboration with Lund University enables characterizing ultrashort light pulses using an unprecedentedly simple and fully inline optical setup, based on recording the optical spectrum of a nonlinear signal produced by the pulse for different amounts of dispersion applied to the same pulse. This results in a 2D d-scan trace from which the spectral phase of the pulse can be retrieved using a numerical algorithm and, therefore, by inverse Fourier transform, provides the exact temporal intensity profile and phase of the pulse. The most common nonlinear signal for d-scan has been second-harmonic generation (SHG) produced in non-centrosymmetric nonlinear crystals. In the present work we use THG as the nonlinear signal. Unlike SHG, THG can be produced in any medium, regardless of its symmetry. Also, for very broadband octave-spanning lasers or mid-infrared systems, it is helpful to use higher-order nonlinear effects, like THG [4]. Here we present several examples of THG d-scan measurements of broadband few-cycle laser pulses obtained in graphene coatings produced by different production techniques [5], which enable characterizing the used ultrashort pulses while providing insight on the electronic dynamics in graphene. The possibility of improving the nonlinear optical response

of graphene and other 2D materials by chemical or morphological functionalization, will also be presented.
This abstract is being submitted as part of a poster presentation.

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Quantum Materials and Quantum Technologies (Posters) / 67

Connecting Stochastic Optimization with Schrödinger Evolution with respect to non-Hermitian Hamiltonians

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In this work, we study the semiclassical dynamics of non-Hermitian quantum systems in phase space. The non-Hermitian semiclassical dynamics of Gaussian coherent states is described by a system of equations for the motion of the center and of the metric associated with the wave packet, which we call the intrinsic geometry of the state [1,2] . The inclusion of a non-Hermitian part leads to the non-conservation of the norm, which can be interpreted as either energy loss or gain. Analytical and numerical methods of solving the dynamics of non-Hermitian quantum systems in phase space are studied and developed. Lastly, a connection is made between the formalism of stochastic optimization of a certain class of control systems and the semiclassical evolution generated by a quantum non-Hermitian Hamiltonian. An example of a quadratic Hamiltonian is explored where we show the existence of the infinite time limit of the center and the metric of the wave packet.

Quantum Materials and Quantum Technologies (Posters) / 68

Localized solutions of the nonlinear Schrödinger equation: application to optics, condensed matter and cold atoms

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Spatial soliton is the wavepacket, which can propagate in nonlinear media without losing its shape due to the perfect balance between the dispersion and the nonlinearity. In this poster we consider solitons as special solutions of nonlinear Schrödinger equation. In its turn nonlinear Schrödinger equation describes various physical systems and objects like matter waves in Bose-Einstein condensate, electromagnetic waves in nonlinear Kerr media, and waves on the surface of deep water. In the poster we consider several examples of solitons in such systems.
As first example we show that vector matter–wave soliton in a Bose–Einstein condensate loaded into an optical lattice can escape from a trap formed by a parabolic potential, resembling a Hawking

emission [1]. The particle–antiparticle pair is emulated by a low-amplitude bright–bright soliton in a two-component Bose–Einstein condensate with effective masses of opposite signs.
As second example we study nonlinear properties of multilayer metamaterials [2] created by graphene sheets separated by dielectric layers. We demonstrate that such structures are described by the discrete nonlinear Schrödinger equation and that its solutions are associated with stable discrete plasmon solitons.
As third example we demonstrate that in an array of nonlinear waveguides, a giant compression of the input beam can be achieved by exciting a Peregrine soliton [3]. Input field almost homogeneously distributed over hundreds of waveguides concentrates practically all the energy into a single waveguide at the output plane of the structure.

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Materials and technologies for Health and Environment / 69

Nanomaterials for Cancer Theragnosis: in silico, in vitro and in vivo.

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Cancer is the second cause of death in Europe and is expected to increase due to the climate changes and population ageing. Early stage detection and effective treatments are keystones to reduce cancer mortality. Nanotechnological systems has been recently demonstrated that are able to perform localized treatment with improved efficiency and reduced side effects. Among the several types of nanomaterials, magnetic and plasmonic nanoparticles are widely used for magnetic hyperthermia and photothermal therapy, respectively, being emergent approaches for thermal treatment of cancer. Nevertheless, although very promising results have been obtained, none of them have yet become part of the standard cancer treatments since thorough challenges must be solved. The successful application of these physically stimulated therapies could be achieved by customization of the magnetic and plasmonic nanostructures shape-architecture, leading to enhanced performance [1, 2].
In this context, the present work shows the development of novel and multifunctional lipid nanoparticles for drug delivery combined with magnetic and near infra-red (NIR) hyperthermia. Superparamagnetic iron oxide and gold nanoparticles were encapsulated in the lipid nanoparticles and used for magnetic and NIR hyperthermia to increase the efficiency of chemotherapeutic compounds [3, 4]. Also results in the field of novel nanostructures for magneto-mechanically induced cell annihilation will be presented from the micromagnetic simulations of high-aspect-ratio magnetic nanowires and vortex nanodiscs, to their surface functionalization, cell internalization, biocompatibility and the preliminary results of in vivo experiments [5, 6].

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Advanced Materials and Processes for Energy (Posters) / 70

Ionic liquid-based fluoropolymer solid electrolytes for lithium-ion batteries

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Population growth and improved lifestyle are responsible for the increase in energy demand. The commitment to renewable energies and batteries for energy storage represent one of the solutions to support continuous energy demands. Lithium-ion batteries (LIB) have the advantage over other batteries with respect to higher energy density by mass and volume, which allows smaller and lighter batteries with high number of charge and discharge cycles. LIBs consist of two electrodes (cathode and anode) and a separator wet in electrolyte. The current electrolyte have important disadvantages, such as being toxic and dangerous for the environment, and present a risk of explosion. Solid polymer electrolytes are among the key issues in future battery technologies [1]. Polymer based solid polymer electrolytes (SPE's) can be defined as solvent-free salt solutions in a polymer host material with high mechanical stability. SPE's consist of a polymeric matrix combined with an ionic conductive filler and its main advantages are safety, long lifetime, low charge time and low internal corrosion [2].
In this work, a novel SPE is presented based on an IL ([BMIM][SCN]) in different polymeric matrix (PVDF and PVDF-HFP). The morphological (Figure 1a), physical-chemical, thermal, mechanical, and electrochemical properties of the composites were studied. Ionic conductivity value, electrochemical window stability and charge-discharge performance of the SPE in cathodic C-LiFePO4 half-cells were evaluated to demonstrate the suitability of the developed composites as SPEs for a new generation of solid-state lithium-ion batteries. It was proven that the developed SPE shows similar results than conventional batteries with liquid electrolytes, with a capacity fade of 16% over 30 cycles (Figure 1b).

New principles and technologies for sensing / 71

Micro/nano sensors for multifunctional applications @ IFIMUP

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Thanks to the development of micro-electronics, sensors can be found everywhere in industry from food engineering to fashion computer design. These sensors can be operating at the complex nature-animal interface, process gigantic volumes of information in real time.
According to MarketandMarket, the Industrial Sensors market will grow from USD 18.2 billion in 2020 to USD 29.0 billion by 2025, with a CAGR of 9.8%. Growing popularity of industrial 4.0 and IoT and increasing demand of industrial robotics are the key factors driving the growth of the market. The development of advanced sensors with multifunction operations are the major goal nowadays. At this session it will be exposed the state of the art at IFIMUP regarding the use of several types of sensors that are being designed and developed by microfabrication techniques or by printing techniques.

The fabricated sensors presented have multiple applications such as thermal, optical, pressure, humidity or even biological applications.

Advanced Materials and Processes for Energy (Posters) / 72

MWCNT-based inks optimization for Textile supercapacitors using screen printing method

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Recently, the demand for intelligent textiles and smart materials is growing in the world motivated by the market requests for innovative high-performance products [1]. Electrochemical energy storage systems like supercapacitors (SCs) are promising technologies to develop smart functionalities on textiles, particularly for the area of health and wellness [2]. Screen-printing has long been used in the printing industry, with the advantage of being a low-cost and scalable process [1].
In the present study, inks containing different MWCNT concentrations (17.5, 26.3, 35.1, 43.9, 52.6 mg mL-1) were prepared to reach optimized screen-printing properties. For all tested conditions, the amount of surfactant, binder, additive and solvent were maintained constant. Interdigital planar TSCs were fabricated by applying PVA-H3PO4 solid-gel electrolyte on top of the interdigitated electrodes.
For all the TSCs, the electrochemical performance was conducted by cyclic voltammetry (CV) and galvanostatic charge/discharge (GCD) tests in a standard two-electrode cell configuration. From the CV curves, a nearly rectangular shape without redox-based humps was observed for all TSCs, proving their electric double-layer (EDL) type behavior.
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Advanced Materials and Processes for Energy (Posters) / 73

Printed Flexible μ-Thermoelectric Devices

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Thin and flexible micro thermoelectric generators (□-TEGs) are being envisaged as alternative power sources in the last decade [1]. They constitute a new business opportunity for the packaging industry such self-powered wearable mobile electronics and/or to be used on remote places for low power consumption devices. One approach to achieve this goal are by producing thin films using composite pastes composed by inorganic material and polymeric matrix to fix onto the flexible substrate. This strategy is the one that unveil better achievements in the last few years and more promising due to low-cost production and the easy to scale up to the market. Bi2Te3 has been recognized as a prime TE material with the best performance values for RT applications. The current challenge is the combination of Bi2Te3 materials with a polymeric matrix towards the production of a printable paste without loss of TE properties [2].

Advanced materials and processes for Energy / **74**

Engineering Ferroelectric Perovskite Oxides with Narrow Band Gap

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The scope of this research line is to investigate a new class of ferroelectric (FE) oxides with tuned band-gap (Eg) to address multiple photovoltaic (PV) key-mechanisms that will enable to develop a groundbreaking approach to the design of solar cells (SC): i) Eg ≤1.5 eV optimized for solar radiance absorption; ii) Non-centrosymmetric structure upholding FE Polarization (P) >50 μC/cm2 and Tc >500 K; iii) Twofold percolative paths for independent transport of e- from h+ to minimize recombination.
The core concept of this project exploits the FE polarization (P) [LV16] to replace the archetypical p-n junctions by-passing barrier losses and enabling power output above Eg, to surpass the semiconductors efficiency limitations. Moreover, the typical resilience of oxides allow to overcome stability issues found on SCs based on organic frameworks. The comprehensive studies and optimization of a series of promising photo-sensitive double-perovskite-like oxides, are based on the formula A2B' B"O6 [DK18]. Systems already under research are Bi2ZnTiO6 [FF19] and Bi2Zn3/2Mo1/2O6 thin films. The R&D strategy involves proactive DFT calculations to run simulations of the materials and heterostructures with asymmetric interfaces to settle P and selective extraction of e- apart from h+. Attention is given to employ feasible thin films deposition methods, like rf-sputtering, standard glass or Si substrates and functional oxide buffers like LaNiO3; MoO3, ZnO and ITO [AM20]. Envisaging affordable, robust, "lead-free"and environmentally friendly all-oxide Solar Cell demonstrator compatible with industrial CMOS fabrication. FE oxides with low Eg have real potential for innovative applications in multi-source energy harvesting, photo-electrochemistry, photo-catalysis and a new opto-electronic actuators or sensors. This project is clearly motivated to contribute for developing energy harvesting processes from renewable and carbon-free sources like Solar; in definite alignment with the UN and EU Global Environmental and Climate Emergency Declarations.

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Scientific Area:

Advanced Materials and Processes for Energy (Posters) / 75

NUMERICAL SIMULATiON OF A PASSIVE THERMAL SWITCH

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Keeping devices operating at adequate temperatures is necessary for numerous technological areas. One innovative component that can contribute to this control is the thermal switch (TS). TSs rely on the switching of thermal resistance between two states: during the "on"("off") state, the thermal resistance is minimized (maximized), thus maximizing (minimizing) the heat transfer. In this work, we simulate the performance of a novel passive thermal switch.

Scientific Area:

Advanced materials and processes for Energy / 76

Tuning Bi2Te3 nanoparticles for high performance flexible thermoelectric nanogenerators

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During the past few decades, with rapid enlargement of human society, consumption of traditional energy has increased exponentially. Thermoelectric materials (TE) can generate electrical energy when they are exposed to a thermal gradient, considered one of the most important solutions for sustainable energy harvesting.[1,2] These materials present lightweight, small size, pollution free and recycling potential.[2] One of the most used TEs is the alloy Bi2Te3 since it is considered as the best performing thermoelectrical material near room temperature (150-300 K).[2] The performance of a thermoelectric material is assessed by a dimensionless figure-of-merit, zT, defined as zT = S2σT/(κe + κl), where S, σ, κe, κl and T are the Seebeck coefficient, electrical conductivity, electronic and lattice thermal conductivities, and the absolute temperature, respectively. An average zT between 1.5–2 can enable substantial waste-heat harvesting and application in primary power generation.[3] Recently, in order to obtain high zT values, was developed Bi2Te3 nanomaterials leading thus a strong quantum confinement and a significant reduction of the lattice thermal conductivity, causing an increase of the zT value.[4]
Herein, it was prepared Bi2Te3 NPs using a chemical reduction process and a polyol to confine the NPs size.[5] The NPs were characterized by XRD, DLS, SEM and transport properties presenting a mix of Bi2Te3 with a small amount of Te, an average hydrodynamic diameter of 261±23 nm (PDI = 0.31±0.04, n = 5), S = +172.8 μV K-1 (being p-type material), σ = 22.20 S mm-1, and a Power Factor of 0.662 μW m-1 K-2.

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Advanced materials and processes for Energy / **77**

Thermally-Chargeable Textile-Based Supercapacitor by Soret Effect

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The Era of the IoT and the paradigm of Sustainable Energy boosted the search for self-powered devices that harvest and store energy to satisfy the electrical needs of the generation of autonomous wearable electronics.1,2 Thermally-chargeable supercapacitors are a clean energy technology that is able to convert the waste thermal energy into electrical energy (as a power source) and, simultaneously, store that energy (as an energy storage system). These hybrid devices allow converting the waste thermal energy provided from low-grade heat sources (e.g., human body) into electrical energy by a thermally-induced migration of electrolyte ions towards the device electrodes based on the Soret effect.1–3
Herein, we report on the fabrication of a thermally-chargeable textile supercapacitor (TCSC) composed of two multiwalled carbon nanotube-coated cotton electrodes (MWCNT@cotton) and an all-solid-state ionic polyelectrolyte (PVA/H3PO4). The MWCNT@cotton electrodes were prepared by directly coating the cotton substrates with a MWCNTs dispersion through a scalable textile industry process. The ionic conductivity of PVA/H3PO4 electrolyte was tuned by doping the PVA matrix with different wt% of H3PO4, unveiling an ionic conductivity value of 39 mS/cm for a PVA/H3PO4 ratio of 1:1 (m/m). The TCSC was fabricated by sandwiching the ionic electrolyte between the MWCNTs/cotton electrodes. The thermally-induced power generation of the TCSC was evaluated, reaching a Soret coefficient of ˜2 mV/K (up to 30 mV for an applied temperature gradient of 25 K). Concerning the energy storage features, the TCSC presented an electric double-layer charge storage mechanism, affording a working voltage of 2.27 V and an energy density of 4.33 Wh/kg at a power density of 620 W/kg. The high flexibility and the efficient performance of the TCSC, combined with the scalable and cost-effective fabrication process, make this device a feasible solution to satisfy the challenges of autonomous wearable electronics.

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Materials and technologies for Health and Environment / **78**

Atomistic simulations of silver diffusion within a titanium nitride matrix

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To mitigate the carbon footprint of aerospace industry, light and high-performance materials are currently needed, however they are very difficult to cut and machine. Self-lubricating coatings represent a way to reduce the wear of machining and cutting tools, hence increasing their lifetimes with clear advantages in terms of environmental sustainability. In this sense, it has been recently shown that TiSiN(Ag) nanocomposite coatings are very promising.[1,2]
In such systems, the diffusion rate of silver within the matrix plays a critical role and needs to be fully understood and controlled.
Here we apply both density functional theory (DFT) calculations and classical molecular dynamics (MD) simulations to gain insight into the transport of silver within TiSiN coatings. The formation energies of defects such as Ag interstitials and substitutions have been obtained with DFT. Bulk TiN, TiN GBs and at the TiN/SiN monolayer interfaces have been considered. Potential energy landscapes were obtained for the diffusion of Ag atoms on free TiN surfaces, as well as along Duffy-Tasker and Kingery type TiN grain boundaries.
MD simulations of TiN/Ag systems to observe the silver diffusion in presence of GBs and surfaces at different temperature and pressure conditions, for which a hybrid MEAM/Mie force field has been developed.[3]
Our results indicate that the diffusion along TiN surface is the fastest diffusion mechanism. Diffusion along grain boundaries is slower and directly related to the size of GB. On the contrary, bulk diffusion appear extremely slow, because of the high formation energy of related defects. Our study provide a clear understanding of the Ag diffusion mechanism in TiSiN/Ag coatings, indicating that the most relevant process is surface diffusion along intergranular space. Hence, acting on this process is the key to tune and improve the coating's performance.

Scientific Area:

Quantum Materials and Quantum Technologies (Posters) / **80**

Phase sequence and dielectric properties of K0.5Na0.5NbO3 ceramics sintered by different methods

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In order to substitute lead zirconate-titanate (PZT) based materials, due to its poisonous nature, some promising piezoelectric and friendly environment compounds are attracting growing attention, namely KxNa(1-x)NbO3 [1]. For the case of x=0.5, K0.5Na0.5NbO3 (KNN), the high-temperature cubic symmetry changes to a non-symmetric ferroelectric tetragonal structure at T3=700 K, becoming orthorhombic at T2=465 K, and finally stabilizing in a rhombohedral symmetry below T1=135 K [2]. Recently, theoretical calculations have predicted piezoelectric response enhancement when T3 become closer to T2 [3], in which sintering conditions could play an important role [4,5].

In this work, we revisit the phase transition sequence and the effect of the sintering process on the structure, lattice dynamics, and dielectric/polar properties of KNN ceramics prepared by conventional sintering, spark plasma sintering, and spark plasma texturing. From a comparative analysis of the overall experimental obtained results, we have observed that the phase transition sequence includes an unreported structural and polar phase at low temperatures, independently on the processing method. Moreover, apparent changes of the stability temperature interval of the different phases have been ascertained. The dielectric strength and the emergence of a dielectric relaxation phenomenon are also noticeably dependent on the processing method, which can be understood as an effect of the different grain size. The results here reported clearly point out towards the possibility to change physical properties following different sintering routes to improve device performance.

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Materials and technologies for Health and Environment (Posters) / 81

Fabrication of FePt Nanowires through Pulsed Electrodeposition into Nanoporous Alumina Templates

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According to the World Cancer Report, cancer is the second leading cause of death worldwide, having been responsible for one-sixth of the deaths globally in 2018 [1–3]. Currently, there exist various oncologic therapeutic approaches, the main ones being surgery, radiotherapy, and chemotherapy [4,5]. However, these are often associated with undesirable side effects, since they do not only kill tumor cells but also affect normal cells in the human body, causing, therefore, unwanted damages to healthy tissues [6]. Consequently, an interest has arisen for developing novel efficient therapies with fewer side effects [7].
In this line of research, a relevant approach involves the targeted delivery of anticancer drugs through the use of biocompatible nanocarriers presenting a dual triggering: treatment and transport/release of the drug at the target tumor site. This work appears in such context. Particularly,

we are developing a novel multimodal generation of targeted nanocarriers, loaded with anticancer drugs and capable of exerting a magneto-mechanical action through a magnetic core. Beyond classic magnetic spherical nanoparticles, we are also interested in fabricating nanostructures with unique spin configurations, via template-assisted nanofabrication and lithography, for this application. Additionally, lipid nanoparticles will be used as a shell due to their biocompatibility, surface properties, high drug payload, and reduced absorption via the lymphatic system, which improves drug bioavailability.
Here, we will present the synthesis approaches to obtain FePt nanowires and Au/Fe/Au multilayered nanodiscs [8]. These last nanostructures were employed in macrophage cell assays with and without PEG functionalization, having been observed that they possess an adequate biocompatibility. Furthermore, it was verified a significant reduction of the nanoarchitectures uptake by the macrophages when they were functionalized with PEG.

Advanced Materials and Processes for Energy (Posters) / **82**

Customization of Thermal Expansion in FeCo Nanowires

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There is a great need to control the thermal expansion (TE) in the technology industry, where devices can be degraded due to differences in TE. Negative thermal expansion (NTE) arises as a key to customize the TE. [1] Recent advances at the nanoscale, more precisely nanomaterials with 1D architecture have revealed that TE is a size-dependent feature. [2] FeCo alloys thin films have been proved to possess both a giant and negative magnetostriction [3] being also are considered invar alloy's [4] owning almost zero TE in the transition from ferromagnetic to paramagnetic [5]. Besides, FeCo alloys have diversified applications such as magnetic recording and catalysts [6], motivating the customization of TE in FeCo alloys at nanoscale.
In this work, we synthesized nanowires (NWs) of FexCox-1 (x=10,50,90) [7] through DC electrodeposition using anodic nanoporous alumina as templates [8]. The latter was produced by aluminium anodization which is a highly efficient method to grow self-organized nanoporous in hexagonal distribution with various dimensions [8]. Three solutions with different ionic concentrations of Fe and Co were prepared to obtain the different stoichiometries [7]. An accurate study of electrodeposition potential was performed for each solution to obtain the most efficient and highest deposition rate. This was possible by adapting the Faraday law of electrolysis to a self-ordered hexagonal nanoporous substrate. The morphological and structural characterization of the obtained FexCox-1 NWs with different diameters was carried out by scanning electron microscopy (SEM) and X-ray diffractometry (XRD), respectively.
Ongoing work includes XRD measurements as a function of temperature to determinate the TE coefficient of the FexCox-1 NWs with different diameters. We intend to model the customization of TE of these NWs by varying the key parameters of stoichiometry, diameter and length.

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Materials and technologies for Health and Environment (Posters) / 83

A machine learning application for the tribological behavior of micro-textured surfaces

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In the automotive industry hydrodynamic lubrication is a concern in most of the machinery where there are two contacting surfaces in relative motion. The optimization of these surfaces through micro-texturing represents a very promising way to reduce friction, in order to achieve enhanced lifetimes and reduced lubricant use. However, it is very difficult to predict these optimal texturing patterns.
We present a very efficient neural network capable of predict the Stribeck curves based only on the micro-texturing pattern while also being able to reproduce the reverse process, in which it generates a set of micro-texturing patterns that reproduce the desired input Stribeck curve.
In order to train this machine learning application, we solved the Reynolds equation to obtain the pressure and cavitation profiles by using an implementation of the iterative inexact Newton implementation (INE) in a finite element method (FEM) framework. The solver code, written in MATLAB, was developed and validated in comparison to known cases in literature and tested with complex problems such as lubricated contacts with arbitrarily generated patterns of dimples/defects, thus enabling the efficient generation of a training data set.
Our approach will allow for fast and accurate predictions of the tribological behavior of micro-textured lubricated contacts, at a fraction of the computational cost required for a direct solution method.

Quantum Materials and Quantum Technologies (Posters) / 84

Ca2MnO4 structural path: Following the negative thermal expansion at the local scale

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Naturally layered perovskites have been studied in the designing of novel functional materials, ranging from superconductors to multiferroics, including the recently discovered hybrid improper ferroelectrics, to materials that exhibit negative thermal expansion [1,2]. Particularly, the Ruddlesden-Popper family with general formula CaO(CaMnO3)n has gained considerable interest, where the combined effect of the perovskite layered structure and the condensation of oxygen octahedral rotations modes, underlie both hybrid improper ferroelectricity and uniaxial negative thermal expansion (NTE) properties.
The oxygen octahedral rotations in Ca2MnO4, the first member of the CaO(CaMnO3)n Ruddlesden-Popper family, are here probed through a set of complementary techniques, including temperature-dependent neutron and x-ray diffraction, combined with local probe studies and ab initio calculations. Long range order based techniques, such as x-ray or neutron diffraction may present difficulties in correlating, with precision, the evolution of octahedral rotations with the thermal change of the Ca2MnO4 expansion properties, either due to a lower sensitivity to oxygen atomic positions, as in x-ray diffraction, or due to the actual condensation of the octahedral rotation modes that propagate with a short structural coherence length within the crystal lattice. Time differential perturbed angular correlation (TDPAC) experiments combined with neutron and x-ray diffraction measurements, and density functional theory simulations provide a unique tool to characterize the Ca2MnO4 structural transitions at the atomic scale [2]. We show that the detailed measurement of the electric field gradient at the Ca-sites, and local symmetry analysis, allow to accurately probe the MnO6 octahedral rotations that underlie the Ca2MnO4 structural transitions and its uniaxial NTE properties.
Here we demonstrate the enhancement of the uniaxial NTE coefficient from -1.26 ± 0.25 to -21 ± 1.8 ppm/K at the second order I41/acd to I4/mmm structural phase transition, providing direct evidence for the recently proposed corkscrew atomic mechanism. We also establish that the aristotype I4/mmm symmetry is attained around 1050 K, a much lower temperature than previously predicted. At lower temperatures, within the 10–1000 K temperature range, our first-principles calculations and detailed analysis of the Ca local environment reveal that the reported Aba2 structural phase, coexisting with the I41/acd one, cannot correctly describe this compound. On the other hand, our data allow for the coexistence of the locally identical I41/acd and Acam structural phases.

Quantum Materials and Quantum Technologies (Posters) / 85

Strain-induced effects of topological deformed graphene

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The dynamics of electrons in graphene can be described by a two-dimensional (2D) Dirac equation. Graphene is a two dimensional material embedded in three dimensions and is assumed to define a 2D flat surface. However, one expects deviations from flatland. Structural corrugations and ripples, have been observed in suspended graphene, and furthermore, atomistic simulations have shown that ripples appear spontaneously owing to thermal fluctuations [1]. Geometric curvature and strain in graphene can give raise to pseudo-magnetic fields which can lead to observable phenomena. Furthermore, it is possible to connect strain with the possibility of opening energy gaps in the graphene electronic spectrum and already experimentally observed [1].
We present an analytical solution of the relativistic Dirac equation defined in the framework of quantum field theory in curved space and apply it to study the electronic properties of deformed monolayer graphene [2]. We obtain as solution the Dirac oscillator equation where an effective vector potential term naturally appears. Such a term describes a pseudo-magnetic field which emerges due to the initially defined curvature, and influences the dynamics of the charge carriers as if these were under the influence of an applied external magnetic field.

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Quantum Materials and Quantum Technologies (Posters) / 86

First-Principles Calculations of Electric Field Gradients in Hf-Based Perovskites: a Tool to Identify Transition Pathways

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We present an ab-initio study performed by means of Density Functional Theory (DFT), group-subgroup symmetry analysis and lattice dynamics to probe the properties of the octahedral distortions, which occur during the structural phase transitions [1]. We mainly focus our study on the Sr3Hf2O7 (SHO) system, which is characterized by a high-temperature I4/mmm (S.G. 139) centrosymmetric structure and a ground-state Cmc21 (S.G. 36) ferroelectric system. We have probed potential candidate phases that may form the I4/mmm → Cmc21 transition pathways, namely Fmm2 (S.G. 42), Ccce (S.G.68), Cmca (S.G. 64) and Cmcm (S.G. 63). We found that the band gap widths increase as the symmetry of the systems decreases, with the ground-state structure presenting the largest gap width (˜5.95 eV). By probing the Partial Density of States (PDoS), we observe a direct relation regarding the tilts and rotations of the O perovskite cages as the transition occurs; these show large variations mostly of the O p-states which contribute mostly to the valence band maximum. We have also computed the macroscopic polarization and confirm that the Cmc21 phase is ferroelectric with a value of spontaneous polarization of 0.0478 C/m2. The ferroelectricity of the ground-state Cmc21 system arises due to a second order parameter related to the coupling of the rotation and tilts of the O perovskite cages together with the Sr displacements.

The measurement of the Electric Field Gradients (EFG) and asymmetric parameters, through hyperfine techniques, i.e. nuclear quadrupole resonance (NQR) or perturbed angular correlation (PAC), combined with ab-initio DFT calculations, has shown to be a valuable tool to probe the octahedral rotations of the cages during phase transition. Therefore, we have computed the EFG for each structural phase and observe variations of respective parameters which allow the possibility to ascertain for the correct phases/pathways, namely the ones connected by group-subgroup relations. In such a way, these techniques can inform about the subtle octahedral tilting and rotations, which are typically not easily accessible by long-range crystallographic techniques.

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Materials and technologies for Health and Environment (Posters) / 87

A study on materials for radiofrequency electromagnetic interference shielding: metamaterials, nanomaterials and textiles

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The continuous developments in radiofrequency electromagnetic (EM) radiation applications such as communication technologies, data transference, wireless internet, automatized electronics, etc., has been consistently increasing EM radiation exposition. For this reason, the scientific community is questioning the impact that EM radiation could cause in the human health or affect electronic appliances operations [1]. To overcome these issues, electromagnetic interference (EMI) shielding has been extensively investigated and applied as a solution.
The EMI shielding field is dominated by the use of metals such as silver or nickel. However, the use of these materials introduces some challenges, namely lack of flexibility, corrosion, high cost or heavy weight. For these reasons, alternative approaches such as the use of carbon materials, conductive polymers, magnetic materials, metal oxides and nanocomposites, have been investigated [2]. Metamaterials for improving other properties such as breathability, optical transmittance and reducing material's usage could also be considered. Textiles are versatile solutions for EMI shielding, for being flexible, lightweight and applicable for clothing, electronic protection, aerospace application, etc.
In this work, diverse materials are considered, namely carbon nanomaterials, conductive polymers, and commercial metallic inks. Different applications techniques in textiles are investigated, such as dip-coating, screen-printing and coating. The EMI shielding properties were measured using an adaptation of the transmission line test including conjoined wave-guides connected to a vector network analyzer (VNA), where the sample is inserted in the middle and the scattering parameters are obtained. It was possible to obtain the shielding effectiveness (SE) in decibel (dB), in the frequency range from 5.85 to 18 GHz. Additionally, a simulation on COMSOL Multiphysics was applied for studying quadrangular metallic meshes.
Promising results were obtained with coatings of PEDOT: PSS and MWCNTs formulations applied over cotton textile substrates, reaching SE considered to be excellent for general use applications and very good for professional applications [3]. Furthermore, results from simulations bring interesting perspectives for reducing material's usage while maintaining similar SE levels.
Submission for poster presentation.

Quantum Materials and Quantum Technologies / 88

The importance of incommensurability in twisted bilayer graphene

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We studied the localization properties of electrons in incommensurate twisted bilayer graphene, for twist angles encompassing the narrow-band regime, by numerically exact means.
Incommensurability effects were found to induce states with sub-ballistic properties in the narrow-band regime. These states are delocalized in momentum-space and follow non-Poissonian level statistics, in contrast with their ballistic counterparts found for close-by commensurate angles.
Transport results corroborate this picture: for large enough systems, the conductance decreases with system size for incommensurate angles within the sub-ballistic regime.
Our results are at odds with the current belief that, for small angles, there are no qualitative distinctions between commensurate and incommensurate structures. In particular, we show that incommensurability effects are of crucial importance in the narrow-band regime and that the incommensurate nature of a general twist angle must be taken into account for an accurate description of magic-angle twisted bilayer graphene.

Advanced Materials and Processes for Energy (Posters) / **89**

Pressure-induced phase transformations of Sr3Hf2O7

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We present an ab-initio study performed by means of Density Functional Theory (DFT) and lattice dynamics to probe the octahedral distortions, which occur during the structural phase transitions of the quasi-2D layered perovskite $Sr_3Hf_2O_7$ compound. Such a system is characterized by a high-temperature I4/mmm (space group n. 139) centro-symmetric structure and a ground-state $Cmc2_1$ (space group n. 36) ferroelectric phase. We have probed potential candidate polymorphs that may form the I4/mmm towards the $Cmc2_1$ transition pathways [1] from which the lower symmetry structural phases may be generated by inducing tiltings and/or rotations of the O octahedral cages. We mainly focus our attention to the Ccce (space group n. 68) structural phase, since it has been experimentally evidenced in systems with similar stoichiometry, i.e. $Ca_3Mn_2O_7$ [2]. This phase may occur through a first-order phase transition when temperature decreases towards room temperature, breaking the center-of-symmetry of the tetragonal phase. By observing the phonon dispersion curves of the Ccce phase [1] we find that the system is dynamically unstable at the given conditions of the calculation (0 K and 0 GPa), evidencing negative phonon modes localized at two of the high symmetry points of the Brillouin-zone (BZ): Γ- and Y-points.

As a continuation of the work done so far in $Sr_3Hf_2O_7$, we apply an external perturbation to study, from a theoretical perspective, the possibility of stabilizing the respective Ccce phase at room conditions. Pressure is an important thermodynamic variable which enables the understanding of the properties of materials, even at room pressure, since it allows for a precise control over the interatomic distances and hence the atomic interactions. We will hence show in this work the variation of the structural, vibrational and electronic properties of the Ccce structure as a function of applied hydrostatic pressure.

Acknowledgements

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Quantum Materials and Quantum Technologies (Posters) / 90

Memristors coupling neurons

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Significant efforts are being made to develop nanoscale electronic devices capable of emulating the dynamics of natural synapses to be integrated into neuromorphic circuits. Furthermore, to couple different neuronal populations via such artificial synapses bears great potential for therapeutic strategies focused on the monitoring and control of neuronal electrical activity. Such hybrid systems, effectively coupling biological and electrical components, are important milestones for the development of a new generation of neuroprosthetic devices aimed to address a number of challenging neurologic disorders [1]. Memristors have gained attention as a core component is these hybrid systems, mainly because of their neuromorphic properties, small size and low power signature [2]. Relevant proofs of concept have already been presented in the literature [3], but we argue that crucial aspects have not yet been demonstrated on how these memristor-based hybrid systems can effectively operate in a meaningful way. Here we show, for the first time, how biological in vitro neuronal populations can be dynamically coupled with a memristive device acting as a synapstor, forming a hybrid bio-electronic system. We demonstrate that the conductance state of a memristor can be changed by the electrical activity of biological neurons and mediate a dynamic connection between isolated spiking neuronal populations. Our system connects biological neurons to microelectrodes, amplifier, memristor, stimulator, microelectrodes, and back to biological neurons, in an effective real-time configuration that does not use software nor simulations (Fig. 1). This allowed us to have the Target neuronal population being effectively activated if, and only if, there is network bursting activity in the Source population. Importantly, we demonstrate that our artificial synapse is capable of short-term plasticity, dynamically changing its conductance level in both directions. Our results pave the way for further implementation of elements able to perform more complex modulatory operations in neuronal populations.
(Fig.1)
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91

Low impedance electrodeposited PEDOT:PSS thin films

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Abstract submission for poster talk on behalf on Henrique Teixeira from IFIMUP.

Advanced materials and processes for Energy / 92

Advanced nanostructures trends on photoelectrochemical cells for solar water splitting, green hydrogen generation

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One of the greatest challenges of the 21st century is to reduce greenhouse gas emissions, while keeping the standard of living, by using more clean and renewable energy sources. Sunlight is by far the most abundant renewable source of energy, exceeding the potential of all other energy sources, and capable of supplying the present and projected world's energy demands. Photoelectrochemical (PEC) cells offer an excellent method of producing both electrical (dye-sensitized solar cells - DSCs) or chemical energy (fuel - H2 production by water splitting) [1]. H2 generation via PEC solar water splitting is a promising approach since it combines the solar harvesting, conversion, and storage functionalities all-in-one, which is favorable in terms of packaging and overall system costs. Materials based on n-type metal oxides such TiO2, α-Fe2O3, or WO3 have gained relevance for such applications due to their low cost, easy preparation, synthesis, and high stability in aqueous media. Nanostructuring has emerged as one of the best tools to enhance the photoelectrodes' efficiency response. Different synthesis methods for preparing nanostructured photoelectrodes with different geometries (e.g. nanoparticles, nanoplatelets, nanopores, nanowires, nanotubes, etc.) have been widely explored to obtain an enhanced efficiency in the photoresponse, specifically by physical, electrochemical, and chemical routes. More recently, a great interest in nanotubes and nanowires geometry has emerged for applications in PECs. We propose to implement the most abundant/low cost and chemically stable, semiconductors oxide materials (e.g. TiO2, α-Fe2O3, WO3) using highly scalable (low cost) synthesis methods: hydrothermal, chemical, and electrochemical anodization processes. We obtained nanostructured photoelectrodes, nanoplatelets, nanowires, or hexagonally-ordered nanotubes arrays of semiconducting oxides for the PEC solar cells applications [2-5]. Detailed characterization and optimization of such nanostructures were made with detail and thoroughness to optimize the photoresponse.

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Materials and technologies for Health and Environment (Posters) / 93

2G4CANCER –Green graphene/lipid nanosystems for cancer imaging and treatment

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Cancer remains a worldwide leading death cause, prompting the necessity to develop new therapeutic solutions [1]. Current cancer chemotherapeutic agents can induce toxicity, even at therapeutic doses, and become ineffective by multidrug resistance (MDR) development. Furthermore, traditional synthesis of treatment and imaging agents promote some undesirable toxicity.

Doxorubicin (DOX) is a "first-line"treatment for different types of cancer which intercalates between DNA base pairs and kills fast-growing cancer cells, while also displays toxicity in healthy tissues [2,3]. Since the first DOX-loaded liposomes were approved for cancer treatment [2], research

focused on these nanocarriers to reduce toxicity to healthy tissues. However, DOX-nanodelivery systems have low therapeutic efficiency due to their limited drug loading capacity, and so, pH or ion gradients are used to massively entrap DOX in the nanocarriers'aqueous core causing aggregation. These aggregates are less effective in DNA intercalation. Furthermore, even when delivered by nanocarriers, DOX is still non-specifically distributed at non-target tissues [2]. 2G4CANCER proposes DOX conjugation with green-graphene oxide quantum dots (2G-QD@DOX), due to their potential in biological labelling, photoluminescence, photostability and biocompatibility thus enabling cancer theranostic applications. The DOX conjugates will further be encapsulated in nanostructured lipid carriers of cubosomal type for higher drug entrapment and reduced oligomerization. For comparison purposes we are also testing cubosomes prepared from hybrid combinations of lipids and polymers to further encapsulate DOX.
In summary, 2G4CANCER proposes the development of eco-friendly biosynthesis of 2G-QD, to be conjugated with DOX and encapsulated in nanostructured lipid carriers to improve biodistribution and allow bio-tracking. DOX@2G-QD nanocarriers will be further silk-coated to promote stability, while allowing conjugation with siRNA for knocking-down cancer MDR pathways. Therefore, the smart nanocarriers proposed hold a multiple concept for cancer treatment: (i) enhanced therapeutic effect, (ii) imaging for traceable drug delivery, (iii) higher selectivity (by incorporating peptides targeting HER2), and (iv) controlled drug release profile.

Materials and technologies for Health and Environment / 94

Health and Environment Research Areas at C2TN

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The research activities at C2TN´s Health and Environment areas are represented in 2 of the 3 Thematic Strands of the centre. In this seminar we will present the activities performed under the Radiopharmaceutical Sciences and Heath Physics (RSHP) thematic area as well as the research in the Earth Systems, Radioactivity and Cultural Heritage (ESRCH) area.
In the RSHP area the scientific program is focused on Radiopharmaceutical Sciences, Radiation Protection and Dosimetry, and on the Biological Effects of Ionizing Radiation and Metrology, in order to contribute to the following major topics: a) design and preclinical evaluation of radiopharmaceuticals for a better management of cancer and neurodegenerative diseases with personalized diagnosis and/or treatments; b) quantification of the risks associated to low dose and protracted radiation exposures and c) assessment of the doses and risks due to the exposure to ionizing radiation of the patients and medical staff, to improve the Quality and Safety of health care.
In the ESRCH thematic area the scientific program takes into consideration the key expertise of C2TN in nuclear techniques, natural sciences and environmental radioactivity, radioactive waste management, actinides, lanthanides and other chemical elements behavior, application of ionizing radiation, radionuclides and stable isotopes to Geosciences, Environment and Cultural Heritage. The research and development activities comprise: (i) identification of major driving factors controlling the Earth surface composition; (ii) environmental radioactivity and radioecology; (iii) radioactive waste management; (iv) characterization of critical and strategic mineral raw materials; (v) identification of pollutant sources in groundwater and superficial water systems; (vi) interaction of ionizing radiation with matter; (vii) identification and quantification of emission sources contribution to air pollution; and (viii) Cultural Heritage –characterization and contribution to the establishment of conservation strategies.

Scientific Area:

Quantum Materials and Quantum Technologies (Posters) / 95

Sputtered topological insulators for Spinorbitronics logic devices

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Spintronics has seen remarkable progress in the last decades. By combining well known concepts like Giant and Tunneling magnetoresistance with spin torques and control of domain walls, developments are foreseen in data storage [1] and logic, with new devices like the magnetoelectric spin-orbit MESO logic device [2]. New materials and nanostructures have also allowed several breakthroughs, from 2D materials to Topological Insulators.
Topological Insulators (TI) are a peculiar category of materials. Having been experimentally discovered only in 2007 [3], they have already shown great promise for a wide range of applications. Due to their performance in the control and switch of nanomagnets based on the Spin Orbit Torque (SOT), they could lead the advancements of new memory and logic devices.
One family of materials that has arisen within TIs is the Bi2Se3 family of semiconductors. They host a metallic state on their surface while having an insulating bulk. The metallic state is protected by time reversal symmetry and presents a spin texture. Moreover, due to their strong spin orbit coupling, high values of the Spin Hall angle θSH have been reported [4], leading to outstanding control of nanomagnets. Sb2Te3 is one of the members of this family, with the TI surface state being theorized in 2009 [5] and later observed [6]. However, it has not been widely studied due to its smaller band gap. Thus, it is not yet clear if it is a material of interest for SOT applications.
In this presentation, ion beam sputtered thin films of Sb2Te3 with thicknesses ranging from 35 to 200 nm are going to be explored. Their transport properties will be presented and discussed. By correlating the magnetoconductance and thermoelectric properties of the sputtered Sb2Te3 thin films, the exotic conduction of these materials will be untangled. Following the characterisation of these TI thin films, bilayers with magnetic permalloy thin films were produced and the current spin to charge conversion studies will be addressed. As the thin films have been made using a scalable inexpensive fabrication method, already employed in the industry, these results shine light into a novel topological insulator, with promising opportunities for future applications in spintronics.

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Scientific Area:

New principles and technologies for sensing / 96

Nanofabrication of Pd and PdAu nanowires in alumina dendrites for hydrogen sensing

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Hydrogen (H2) fuel is emerging as one of the most viable green solutions in response to the rising global energy consumption. However, due to its high flammability, H2 can cause severe explosions in case of leakage [1]. Several H2 sensors have been developed, and palladium (Pd) based sensors have shown important optical and electrical properties, with the ability to dissociate catalytically the H2 molecule at its surface, by incorporating the resulting H atoms into its crystalline structure [1]. The use of nanostructure Pd–alumina metamaterials can highly improve the sensing properties, such as increased optical sensitivity to H2, improved sensor´s repeatability and durability, and can provide a route to tune the H2 absorption and desorption rates, that limit the H2 sensor response and recovery times [1,2]. Still, pure Pd based H2 sensors may inherently display non-linear behavior and large response times (on the order of minutes), while the use of PdAu alloys allows to suppress H2 absorption-desorption hysteretic behavior and decrease the sensing response times down to the order of seconds [3].
In this study, we review the fabrication of metamaterials for H2 optical sensing applications based on Pd/PdAu nanowires (NWs) and dendritic nanostructures grown inside nanoporous anodic aluminum oxide (AAO) templates by pulsed electrodeposition (Fig. 1). First, AAO templates were produced through an electrochemical anodization self-assembly process, where the controlled conditions allow tuning the diameters of the pores and result in hexagonal-close-packed arrays with dendritic nanostructured terminations [4]. The H2 optical response of homogeneous Pd NWs, in the order of 127 nm length and 49 nm diameter decreasing up to ˜13 nm, as dendritic generations are formed, is reviewed [1]. To improve sensing performance, nanostructured PdAu alloys were fabricated, where the alloy composition was adjusted from 5.65-25.5 at.% Au by a simple change of the applied current density from 15-50 mA·cm-2 in the electrodeposition process. Future tests will include the use of the prepared PdAu-based metamaterials in a homemade optical fiber sensor device.
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Scientific Area:

Materials and technologies for Health and Environment (Posters) / 97

Multimodal magnetic lipid nanocarriers for cancer therapies

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The advances made on the field of nanotechnology have brought a variety of new possibilities into drug discovery and medical therapy [1]. In this context, nano-scaled carriers have revolutionized drug delivery systems, allowing for therapeutic agents to be selectively targeted to a specific tissue, thus decreasing exposure of healthy tissue to drugs. Nanostructured lipid carriers (NLCs) are the second generation of lipid nanoparticles, which have been drawing much attention of researchers due to their safe and biocompatible features [2]. Additionally, their low cost can boost their translation from the bench to the bedside. Particularly, NLCs have several advantages when compared with other lipid drug delivery systems (for example liposomes or niosomes), such as, great kinetic stability, stable morphology and high load capacity. In this work, we developed, physico-chemically

characterized and tested in vitro, two distinct NLCs formulations, for the targeted delivery of an anticancer drug –Doxorubicin (DOX). The overall results are very promising, however the combination with magnetic nanoparticles (SPIONs), nanowires and nanodiscs, developed in a parallel study, may further improve the therapeutic index of the formulations. The strategy of developing core-shell structures with a predefined set of hierarchical functionalities allows magnetic nanoparticles, nanowires and nanodiscs to be used in multipurpose applications that can simultaneously provide magnetic resonance images, enhanced drug delivery and hyperthermia by magnetic excitation. Hence, these hybrid nanoparticles should lead to negligible systemic and reduced side effects of DOX.

Quantum Materials and Quantum Technologies (Posters) / **98**

Statistical Analysis of Photoluminescence Decay Kinetics in QD ensembles

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Semiconductor quantum dots (QDs) are considered ideal building blocks to produce materials with specific photonic and spectroscopic properties. The possibility of controlling their properties such as size and doping during preparation facilitates the fine tuning of their optical properties such as absorption and emission spectra. The optical properties of QDs are affected by their environment via energy and possibly charge transfer processes between the dots and surrounding materials. Time-resolved single photon counting (TCSPC) of the photoluminescence (PL) decay is a key experimental method used to characterize the excited state dynamics and explore these effects, having become a well-established quantitative tool.

However, understanding and modelling the fluorescence lifetimes obtained via TCSPC is far from straightforward. The main difficulties are that the QD systems are heterogeneous and the overall fluorescence decay is influenced by several different mechanisms. One such mechanism is the Förster Resonant Energy Transfer (FRET) that can take place for different environments including other QDs.

In this work we present two methods of statistical analysis of the decay kinetics using (I) the probability distribution function (PDF) and (II) statistical moments. Both methods reveal FRET occurring in a mixture of QDs of two different sizes and, specially, the latter can be more informative in terms of donor-acceptor spatial correlations.

Advanced materials and processes for Energy / **99**

H2 Solar: Thin films multilayers of semiconductors oxides for photoelectrochemical water splitting

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The global energy consumption has been sharply raising over the years. To sustain the energetic needs and simultaneously combat the harmful use of pollutants, it is necessary to resort on efficient green energy sources with the possibility of storing their products. Photoelectrochemical (PEC) cells relies on semiconductors to convert the absorbed solar light into green hydrogen through a process of photogeneration of electron-hole pairs which chemically splits the water molecule [1], producing hydrogen that can be stored, transported, and used as fuel. Several semiconductors (SC) have been extensively studied for PEC cells applications, including SC oxides such hematite, TiO2, WO3, etc. [2]
Following the need for the development of a low-cost, stable, and non-toxic photoanodes [3], the present work resorts on the combination of both, hematite (α-Fe2O3) and titanium dioxide (TiO2) semiconductors. Different photoanodes consisting of Fe and Ti thin films multi-layers were prepared by ion-beam deposition with different thicknesses and arrangement to study these features impact in the final photoresponse. Additionally, thermal annealing optimization was performed where the addition of a high temperature annealing step of 800 ºC for 20 minutes to the first step at 550/600 ºC for 2 hours revealed to be crucial in the photocurrent output.
Photoelectrochemical performances were evaluated by photocurrent density-voltage (J-V) characteristic curves in the dark and under 1 sun AM 1.5G illumination. The morphological and structural characterization of the obtained multilayers photoanodes was carried out by scanning electron microscopy (SEM) and X-ray diffractometry (XRD), respectively.
Enhanced J ≈ 0.7 mA/cm2 at 1.45 VRHE was obtained for the thin film photoanodes consisting of an FTO/α-Fe2O3/TiO2 multi-layer, i.e. TiO2 layer in the top of the α-Fe2O3. Additionally, through an analysis of the XRD data, this photoanode presented an increase on the grain size when compared with FTO/α-Fe2O3 or FTO/TiO2 /α-Fe2O3.
Thus, the combination of optimized annealing, semiconductor order and thickness are key parameters to take into account for a highly improved photocurrent, being an indispensable approach to obtain highly efficient PEC cells.

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Scientific Area:

Advanced materials and processes for Energy / 100

High Power Laser Powering Radial Thermoelectric Devices: an innovative Wireless Energy Transfer System

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Nowadays, mobility, convenience, and safety of electronic devices are concerns present in our day-to-day life. Considering that everyday life small devices have a low-power consumption (mW or nW), the search for simple alternative energy sources is rapidly increasing. Energy Harvesting (EH) technology emerges as an excellent solution for this type of application, replacing batteries and providing a long-term power supply [1].

Herein, we propose a new Wireless Energy Transfer (WET) system for long distances, where the most common solutions based on magnetic induction are less efficient. This system combines the concept of WET with EH technology, i.e., thermoelectric generators (TEG) charged by a high-power laser beam. The resulting heat caused by the focused laser beam works as the heat source for the TE device, thus creating a temperature gradient. With sustainability and cost-effectiveness in mind, screen-printing, a low-cost and scalable method, was used to fabricate the TE devices, printed in a flexible substrate, by combining TE particles and a polymeric binder to form the printable ink. The studied inks were formulated using Bi-Te particles (<50 μm) as the functional TE material and Polyvinyl Alcohol (PVA) as the binder, as produced in a previous study [2]. The proposed device presents a radial configuration where the TE stripes are connected in series, and the temperature gradient is applied from the centre (where the laser beam is focused) to the outside. The fabricated devices were characterized at low pressure (˜10^{-6} Torr), reaching a maximum output voltage of 85 mV, with an applied temperature gradient of approximately 80 K. A maximum power density of ˜ 1.1 μWcm^{-2} was attained.
This promising technology can generate a constant voltage for several hours without additional heat dissipation, besides having a rapid response to the incidence of the laser beam. Therefore, it can be advantageous for energy generation in remote places where the replacement of batteries is an inconvenience, and the wireless charging inductive systems fall short due to the long distances.

Acknowledgments
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Advanced Materials and Processes for Energy (Posters) / 101

Combined Density Functional Theory and Perturbed Angular Correlation Study of SrMnGe2O6 and CaMnGe2O6

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Multiferroic materials have been under the spotlight due to their fundamental scientific interest and for potential applications in technology. Among these interesting materials are the group of compounds belonging to the Pyroxene family with general chemical formula AM(Si,Ge)2O6. More specifically, SrMnGe2O6 [1] and CaMnGe2O6[2] are isostructural, crystallizing with monoclinic C2/c symmetry and are characterized by zigzag chains of MnO6 octahedra linked by edge-sharing, separated by GeO4 tetrahedra chains along the same axis, linked by corner-sharing. Due to this arrangement these systems present a rich diversity of low-dimensional magnetic properties. The existence and possible interplay of low dimensionality and magnetic frustration results in multiferroic and/or magnetoelectric properties.
Since these properties might arise from local structural features that are not well described by methods based on long-range average structural models, the use of local probe studies is essential. In this context, hyperfine methods, such as perturbed angular correlation (PAC) spectroscopy where the study of the electric field gradient (EFG) in the vicinity of a probe atom, allows reconstructing of the atomic and electronic environment of the probe in the material, helps to clarify the origin of the properties exhibited in these systems. In this work a temperature dependent EFG study will be presented and discussed, guided by EFG simulation results using ab-initio and WIEN2k [3] and Quantum ESPRESSO [4], attempting to clarify the nature of the two distinct local environments that are experimentally observed in these compounds.

Advanced Materials and Processes for Energy (Posters) / 102

Metal ion exchange mediated structural modulation in layered perovskites: Step towards next-generation energy-efficient materials

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An important challenge of this century is to focus on the production of renewable and sustainable energy, which thrives on research in the development of photovoltaic (PV) materials [1] (solar energy to electricity) and photoelectrochemical (PEC) water-splitting materials (solar energy into chemical energy) [2]. Among the various PV and PEC materials, perovskite structured oxides (ABO3 where A=alkaline or rare-earth metals; B=transition metals) are promising candidates because of their structural and compositional flexibility, excellent stability, and superior optical and electrical properties. Compared to normal perovskites, the layered derivatives show superior photocatalytic performance because they facilitate charge separation due to their unique flexible layered structures. Layered perovskites consist of a perovskite block (ABO3) of varying unit cell thickness n sandwiched between metal oxide layers to form a natural superlattice such as (i) Ruddlesden Popper (RP), (AO)(ABO3)n -alternating perovskite slabs displaced by (1/2,1/2) translation or (ii) Dion Jacobson (DJ), M+1A(n-1)BnO(3n+1) - displacement of the perovskite slabs is either (1/2,0) or is absent. Also, the octahedral rotations or tilts associated with the disconnected octahedra in layered (n = 2) compounds cooperatively give rise to a net polar symmetry with macroscopic polarization known as hybrid improper ferroelectricity (HIF) [3]. In the layered perovskites, the DJ phases offer feasibility for structural modulation via cation-exchange reactions, which stabilizes most metastable phases, which are unpreparable by the direct synthesis routes. In the present study, a series of n = 2 DJ oxides RNdB2O7 (R=Rb, Cs, Na, K and B=Nb, Ta) has been synthesized. (Rb,Cs)NdNb2O7 and (Rb,Cs)NdTa2O7 were synthesized using solid-state reaction, whereas NaNdTa2O7, KNdTa2O7 were obtained by cation-exchange reaction (Fig. 1). The synthesized compounds were analyzed through powder X-ray diffraction. Dion–Jacobson perovskites can also facilitate exfoliation into 2D nanosheets, and finally, the layer-by-layer engineering of 2D perovskite nanosheets has a great potential for next-generation energy-efficient devices [4].

Fig. 1 Cation Exchange in DJ compound

New principles and technologies for sensing / 103

Polarimetry for material characterization in remote sensing applications

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When an optical beam interacts with matter its polarization state can change as a function of certain properties of the material (refractive index, surface roughness, ⋯) and the beam characteristics. Therefore, small differences in such properties can cause the material to reflect or transmit the same

polarized incident beam differently. Consequently, measurements of polarization can be used as a technique to characterize materials. The information provided by polarization techniques can enable accurate studies of a variety of sample condition properties (existence and orientation of surface defects, stress patterns, coating microstructure, ⋯) and it can provide an additional degree of freedom in order to remotely obtain further information about samples.
Polarimetry is the name for a family of optical methods based on measurement and interpretation of the polarization of electromagnetic waves. In order to measure, visualize, and utilize this polarization information, polarimeters are needed. Polarimetry has a strong potential for remote sensing applications. In particular, the information about the sample obtained via polarization measurements could be used for material characterization when considering anisotropic or depolarizing samples. In this context, we are studying the benefits of introducing polarimetric techniques to enhance the detected information and to improve the accuracy of material recognition in order to develop new types of sensors.
In this presentation, I will present a brief overview of polarimetry and the phenomenological reasons for designing polarimetric sensors. Also, I will describe the polarimetric facility developed at the CF-UM-UP and the benefits of introducing polarimetric techniques to expand the volume and nature of the acquired information. In particular, I will focus on the use of polarimetry for increasing material recognition performance.

Scientific Area:

Quantum Materials and Quantum Technologies / 104

Ultrafast Magnetization Dynamics in Multilayered Films Down to the Few-cycle Regime

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Since the first demonstration of the possibility of manipulating the magnetization using femtosecond (fs) laser pulses performed by Beaurepaire et al. in 1996 [1], time-resolved pump-probe measurements based on the magneto-optical Kerr or Faraday effects have provided an invaluable tool for the study of ultrafast magnetic dynamics in many relevant systems [2]. Although rapid advances in ultrafast optical methods have allowed the temporal resolution to be gradually improved, the measurements are routinely performed with few tens of fs (e.g., 30-50 fs). Therefore, achieving a higher temporal resolution is very important for studying ultrafast processes in matter, such as the spin-orbit coupling, the exchange interaction, the structural anisotropy of the materials, among others. With this in mind, we have developed a unique compact versatile time-resolved magneto-optical (TR-MO) system to study ultrafast magneto dynamics processes. Our setup uses state-of-the-art ultrafast optical methods to deliver ultrashort laser pump and probe sub-5-fs carrier-envelope phase (CEP) stabilized pulses at the sample position, permitting the observation of ultrafast magnetization dynamics at unprecedented optical temporal resolutions. This few-cycle regime is also highly promising for the direct excitation and observation of coherent ultrafast magneto dynamic behaviour [3]. Using our TR-MO system we performed magnetization dynamics measurements of [CoFeB/Pd] multilayer thin films in different temporal regimes, as precessional motion [4] and ultrafast demagnetization (Fig.1).

Materials and technologies for Health and Environment (Posters) / 105

Multifunctional Fe-Au nanostructures for biomedical applications

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Cancer is the leading cause of death in Europe after cardiovascular disease, accounting for about 20% of deaths in the European Union [1]. One of the main strategies followed in oncology has been hyperthermia, which consists on raising the temperature of cancer cells to 40-45ºC to reach apoptosis i.e., programmed cell death [2]. One way to reach local and controlled hyperthermia is via functionalizable nanostructures that are activated by external stimuli such as magnetic fields or electromagnetic radiation. Gold nanostructures (Au-NS) have been the subject of much attention in the academic and clinical environment due to its biocompatibility and high absorption of electromagnetic radiation in the near-infrared (NIR) range caused by its surface plasmon resonance [3]. In parallel, magnetic nanostructures based on Iron (Fe-NS) have also been the subject of studies since they can combine the diagnostic properties (as contrast agents for magnetic resonance imaging) and therapy (magnetic hyperthermia) [4]. Although the Fe-oxide NS are the most reported in the literature, Fe-NS are a promising alternative. The high magnetic moment of Fe-NS that can increase the heat dissipation phenomena produced by the magnetic hysteresis, due to the irreversible magnetization/demagnetization processes induced by an applied alternating magnetic field [5].
The main goal of this work is to combine the "best of both worlds"producing multifunctional Iron-Gold nanostructures (Fe-Au-NS) with high heating performance when stimulated with radiation (500-1000nm) and with alternating magnetic fields for applications in controlled and localized hyperthermia.
Fe-Au-NS were produced by two methods: 1) through the ablation of Iron and Gold targets with a femtosecond pulsed laser in liquids (such as ethanol) and 2) by electrodeposition in self-organized alumina matrices. The first technique is particularly interesting for the development of NS-Fe-Au with complex structures such as the core-shell structure [4]. In turn, the second technique allows a controlled growth of nanowires, nanotubes, and more complex morphologies such as segmented Fe-Au-Fe nanowires [6].
The Fe-Au-NS have been fully characterized with scanning electron microscopy (SEM), X-ray diffraction (XRD) and superconducting quantum interference device (SQUID) techniques. The morphological analysis showed a narrow distribution in diameter and length of the obtained structures with improved robustness and high yield, making these techniques versatile approaches strongly compatible with large scale production. Finally, we show the possibility to tune accurately the size of the nanostructures and consequently provide an easy control over the magnetic properties of these nanostructures ultimately enabling reaching the superparamagnetic regime.

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106

Mechanosynthesis of Calcium Phosphates for Additive Manufacturing of Nanostructured Scaffolds

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Biomaterial scaffolds are commonly used to heal bone defects. For Bone Tissue Engineering (BTE), an ideal scaffold must be biocompatible, progressively biodegradable and mimic the structural and biochemical properties of bone [1]. Calcium phosphates (CaP) bioceramics, and in particular hydroxyapatite (HA), adequately meet such requirements and are thus selected for numerous biomedical applications [1].
This project aims to produce multiscale scaffolds for BTE from biogenic calcium-rich raw materials (chicken eggshell (Fig. 1), cuttlefish bone and other bivalve shells), processed via mechano-synthesis with H3PO4 and H2O. The obtained CaP mixtures are used to produce polymer-matrix-composite extruded filaments which feed the additive manufacturing process to yield 3D structures. The design of these structures is outlined and modeled by Finite Element Analysis. Subsequent selective dissolution of CaP forms a nano/submicropore network essential for scaffold's osteointegration and cell migration.
The 3D multiscale design and the biogenic origin of CaP are expected to elicit responses analogous to mechanical and biochemical stimuli as well as more closely emulate natural bone's hierarchical structure, leading to superior scaffold performance.
Studies were conducted to build milling maps for chicken eggshell (calcite) and cuttlefish bone (aragonite) as calcium carbonate sources [2]. Both systems yielded monophasic crystalline HA above milling energy values that depend on the calcium carbonate polymorph used and on H2O content, without any further treatment [2]. These initial results demonstrate the potential of aforementioned biogenic calcium-rich raw materials as natural precursors to produce HA and of high-energy milling as the corresponding processing route, representing an important step towards the production of the proposed enhanced scaffolds.

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Materials and technologies for Health and Environment (Posters) / 107

Towards the magnetic properties of Fe nanowires for biomedical applications

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Recently, a considerable effort has been placed on the study of 1D nanostructures, such as nanowires, nanopillars and nanorods, owing to their biomedical applications [1]
Among several methods that can be employed in the synthesis of NWs, template-assisted electrodeposition in porous anodic aluminum oxide (AAO) has been considered a convenient technique, because of its simplicity and easiness of controlling the size and shape of the nanostructures without requiring expensive equipment or time-consuming processes. AAO templates allow the fabrication of large area and highly ordered nanostructures. In particular, the magnetic behavior of ferromagnetic NW arrays grown in AAO templates has been extensively investigated during the last two decades [2]. Multilayered NWs, built by several magnetic and nonmagnetic materials, have been study by several authors because of the possibility to restraint the magnetic interactions and tune the magnetic anisotropic effects by changing the deposited material and/or the segment lengths [3], having been demonstrated highly tuneable and suitable to the required application. However, with the aim of employing such structures in biomedical applications, and since some metals possess associated toxicity levels, such as Co and Ni, the need to fabricate completely biocompatible segmented NWs have arisen. In this framework, few studies have been reported yet.
Therefore, the main purpose of the present work is the synthesis and characterization of Fe/Cu multisegmented NWs grown by electrodeposition in AAO templates. We have investigated the magnetic behavior of multi-segmented Fe/Cu NWs by varying the number of bilayers from 1 to 20, for fixed Fe and Cu lengths, or changing the magnetic layer thickness for two Cu layer lengths (60 and 120 nm). In this latter case, the lengths of the Cu segments have been accurately chosen to be ≥ 60 nm, corresponding to a situation where the magnetostatic coupling between nanosegments can be neglected. In addition, the Fe lengths have been substantially varied (from 20 to 345 nm) to comprehend the magnetic properties of the nanostructures when increasing their related aspect-ratio. Preliminary studies regarding the cell viability and uptake assays of these Fe NWs were performed in a human breast cancer cell line (MDA-MB 231).

Quantum materials and quantum technogies / **108**

CeFEMA's Research on Quantum Materials and Quantum Technologies & Integration with LaPMET's Strategic Plan

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Since its formation in 2014, CeFEMA has maintained a main focous on Quantum Materials. In this talk, I will describe the lines of research we have pursued during the last few years, the results he have achieved, and the collaborations we have fostered. Next, I will discuss how our research plans integrate with LaPMET's stategy and propose some directions to continue stengthening this reseach line.

Scientific Area:

Quantum materials and quantum technogies

Quantum Materials and Quantum Technologies (Posters) / **109**

Ab initio calculations on cadmium-based multiferroics

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In multiferroic systems, the coupling between electric and magnetic properties gives birth to new tactics to conceive novel technological architectures. The mechanism of ferroelectricity is crucial to materials with high magnetoelectric coupling. As a result, the discovery of hybrid improper ferroelectric (HIF) materials opened new routes for multiferroics design. The Ruddlesden-Popper (RP) and double perovskite (DP) structures are possible HIF compounds, and the RP Ca3Mn2O7 is a prototype for the construction of new HIF materials.
Recently, perturbed angular correlations (PAC) spectroscopy combined with density functional theory (DFT) calculations depicted the relations between the electric field gradient and the structural phase transitions in Ca3B2O7 (B = Ti, Mn) systems. PAC experiments used 111mCd probes that, because of the similar ionic radii and same cation valence charge as Ca, easily substitute Ca ions in Ca3B2O7. Theoretical calculations have shown that Cd is stable at the rocksalt site of Ca3B2O7, leading to the question of how much Cd can Ca3B2O7 incorporate.
Here, we used ab initio calculations to investigate the effect of substituting Ca by Cd in several RP and DP systems. Our results show that enthalpy relations favor the decomposition of Cd-based RP compounds, indicating that experimental synthesis may be nontrivial. Although pure Cd-related RP compounds are not stable, RP Ca3B2O7 (B = Ti, Mn) systems admit the incorporation of certain percentages of Cd replacing Ca. Having a significant impact on the ferroelectric properties, these chemical substitutions can be used to engineer RP and DP materials, increasing their applicability range as ferroelectric and piezoelectric materials [1,2].

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Scientific Area:

Quantum materials and quantum technogies

Materials and technologies for Health and Environment / 110

Advancing supramolecular peptide-based magnetic gels towards smart drug delivery systems

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Peptide-based hydrogels provide many advantages for drug delivery, such as low critical gelation concentration, easy tailoring and modulation, and biocompatibility [1]. The self-assembly gelation

potentiates novel fabrication strategies and the encapsulation of different composites, such as magnetic nanoparticles and liposomes [2]. The combination with magnetic and/or plasmonic nanoparticles provides a means for on-demand drug release, which can be further optimized through the combination with liposomes. These storage units enable the compartmentalization of various drugs that can be released in a sequential and on-demand manner through the use of different triggers [3]. However, the implementation of a stimulus can often lead to undesirable effects on the gel's properties or affect the drug encapsulation.
From the understanding of drug encapsulation in peptide-based gels [4], the use of photothermia as a trigger [5], and the way different nanoparticle functionalization impact the properties [6], peptide-based magnetic gels have progressed towards the combination with liposomes as storage units [6]. Currently, a strategy was developed that enabled the modulation of the chemotherapeutic drug doxorubicin release through the co-assembly of different composites in dehydropeptide-based gels (figure 1). The interplay of liposomes as storage units and nanoparticles co-assembly enabled the tuneability of both passive and active doxorubicin release through different triggers, which makes this design strategy promising for future developments on the control of drug release.

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Materials and technologies for Health and Environment / 111

Nanosystems for magnetic hyperthermia and local drug administration

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In this work, drug-delivery nanosystems with a combination of chemotherapy and magnetic hyperthermia using doxorubicin-loaded magnetic lipid carriers were investigated. The superparamagnetic iron oxide nanoparticles (SPIONs) and doxorubicin (DOX) were encapsulated in two types of nanostructured lipid carriers (NLC): gelucire-based NLCs (NLC(GEL-DOX-SPIONs)) and palmitate-based NLCs (NLC(PAL-DOX-SPIONs)) by a hot ultrasonication method [1]. The SPIONs and DOX alone were synthesized and encapsulated in NLCs for comparison. The resultant magnetic NLCs with DOX-loaded present a hydrodynamic diameter around 200 nm determined by dynamic light scattering (DLS). The structural, magnetic and morphological properties of the nanocarriers were studied by X-ray diffraction (XRD), transmission electron microscopy (TEM), superconducting quantum interference device (SQUID) and optical microscopy. The hyperthermia behavior of free SPIONs and nano-formulations were studied. Drug release tests were carried out in both physiological (pH 7) and tumor medium (pH 5) with a water bath from 35°C to 50°C, and also under an alternating magnetic field (10 mT, 556k Hz). The in vitro cytotoxicity assays in breast tumor cells (MCF-7) indicated that both lipid-based formulations were thermal and pH- sensitive, which allowed a passive drug release under different environments. The DOX-loaded NLCs demonstrated a greater cytotoxic capacity in tumor cells than the free DOX molecule. This therapeutic effect was even amplified in the presence of SPIONs upon an external alternating magnetic field (magnetic hyperthermia). This nanoplatform has been proved to be a promising system in multifunctional cancer therapies combining heat release and local chemotherapy.

Scientific Area:

Quantum Materials and Quantum Technologies / 112

What can Computers Tell us about the Quantum Mechanics of Disordered Electrons?

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Most of our knowledge on the quantum physics of electrons in crystalline matter is based on Bloch's Theorem [1]. This important result states that electrons move like plane-waves across any spatially periodic potential and forms the basis of the electronic band theory of solids. Despite its success in explaining most properties observed in real-life conductors and semi- conductors, exceptional phenomena are known to be caused by (the ubiquitous) deviations from a perfect crystalline order. Paradigmatic examples of disorder-controlled physics phenomena can be traced back to the proposals of P. W. Anderson [2], who discovered that disorder can induce metal-to-insulator transitions caused by localisation of eigenstates [3]. Over the years, many other examples where found, from the emergence of sample specific mesoscopic current fluctuations [4] to the quantised Hall effect in two-dimensional electron gases [5].
In this talk, I will briefly review important disorder effects in both static and transport properties of materials, providing some guidelines on current research trends in the subject [11-12]. The "mantra" of this presentation will highlight the central role of computer simulations in the investigation of disorder effects in condensed matter. This fact will be illustrated by specific examples off some recent work [6-12] done within the condensed matter theory group of CFP. Some of these results share strong ties with the ongoing development of theQuantumKITE [6], an open-source software capable of an exceptionally efficient numerical study of non-interacting disordered quantum matter.

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Quantum Materials and Quantum Technologies / 113

Detecting phase transitions in- and out-of-equilibrium via single-particle covariance matrices

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In this poster we address the problem of detecting phase transitions without prior knowledge of a suitable order parameter. To this end, we propose a notion of metric based on the distance between single-particle covariance matrices. Unlike the well-known fidelity susceptibility, this quantity is accessible to commonly employed numerical techniques and can potentially serve as a versatile instrument to identify phase transitions beyond Landau's paradigm.

In particular, we demonstrate that one choice of metric, which we dubbed single-particle affinity and that coincides with the fidelity for quadratic models can identify non-equilibrium phase transitions. This is shown for a boundary-driven fermion chain under the Markovian dissipation, that escapes Landau's framework. We also apply this method to a fermion ladder and find a rather rich phase diagram, contrary to what would be expected from preceding related work on spin ladders.

Scientific Area:

Advanced Materials and Processes for Energy (Posters) / **114**

Understanding membrane processes on direct liquid fuel cells

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This work intends to develop a theoretical model for the membrane processes on direct liquid fuel cells, particularly the direct borohydride-peroxide fuel cell (DBPFC), as a first step to create a numerical model. The DBPFC is based on the anodic oxidation of sodium borohydride (NaBH4) in alkaline solution with the simultaneous cathodic reduction of hydrogen peroxide (H2O2) in acid media. As the DBPFC uses both fuel and oxidant solutions that are liquid at room temperature, it is a promising device for power generation in space and underwater applications, where O2 gas is not easily available. Crossover through the membrane, specifically in the case of high pH-gradient between the solutions involved, is a crucial point to improve the performance of these fuel cells. Understanding the ion transfer through cation-exchange membranes (CEMs) and anion-exchange membranes (AEMs) will allow the development of pH-gradient-enabled microscale bipolar interfaces (PMBI) [1]. The model is mainly based on the Nernst-Planck equations, where all components of the system are considered to explain the passage of the ions through the membrane used. The latter is split into one section where there is a constant electric field due to the potential difference between the electrodes, and another section without it, but where there is a local difference of electric potential between the two sides of the membrane, i.e., the membrane potential. This effect is created by the different diffusivity of the ions inside the membrane. To keep the electroneutrality in the fuel cell compartments, the system uses a mechanism where the faster ions are slowed down and the slower ions are accelerated, to allow both oppositely charged ions to pass. The passage of the ions is considered individually for each species involved. Each sub-system is considered to work independently based on the different concentrations on each side of the membrane and the specific membrane potential created. The total membrane potential is the overlayed effect of all sub-systems, according to the superposition principle. This model is an upgrade to the generally accepted approach where specific kinds of ions are blocked/hindered by the ion-selective membrane [2]. The obtained experimental data will allow for a better understanding of the processes occurring inside the DBPFC membrane, which has been used until now as a black box, where the initially selected inputs lead to obtaining the polarization and the power density curves as outputs. So far, numerical models for fuel cells have been mainly used for gaseous flows involved, as in the well-studied PEMFC, but a working numerical model for liquid fuel cells is not available in the literature. This study aims to be a starting point to the creation of a corresponding model where liquid solutions are involved, and thus suitable for modeling DBPFCs.

Scientific Area:

Advanced materials and processes for Energy

Advanced materials and processes for Energy / **115**

Ongoing Research in CeFEMA on Advanced Materials and Processes for Energy

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This keynote talk will briefly present the ongoing research in the Center of Physics and Engineering of Advanced Materials (CeFEMA) on the topic of Advanced Materials and Processes for Energy. The CeFEMA team members working in this topic come from the following groups: MemChem - Membranes, Chemical and Electrochemical Processes Group; LASYP - Laser-Assisted Synthesis and Processing Group; NanoMatter - Multiscale Nanostructured Materials Group; and CFNMRS - Complex Fluids, NMR and Surfaces Group.
The research topics include: electrochemical characterization of membranes and electrocatalysts for direct liquid fuel cells (BOR, EOR, ORR, HPRR) and for alkaline water electrolysis (HER, OER); developing membrane processes for attaining significant energy savings (compared to traditional processes) in industrial applications; developing 2D TMDs, i.e., two-dimensional transition metal dichalcogenides, for solar spectrum related applications, e.g. solar cells and photoelectrochemical cells for water splitting; mechano-synthesis of low lithium tin alloys for nuclear fusion applications; and the development of thin films of SnS for photovoltaics, specifically using microwave transient reflection in annealed SnS thin films.

Scientific Area:

Advanced materials and processes for Energy

Materials and technologies for Health and Environment / **116**

Advanced Materials and Technologies for Health and Environment: research studies and collaborations carried out at the Center of Physics and Engineering of Advanced Materials (CeFEMA)

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This presentation will address the studies on Advanced Materials and Technologies for Health and Environment carried out by researchers at CeFEMA, namely for the efficient production of drinking water, the development of biosensors and medical devices which provide support for vital organs such as kidneys and lungs, the provision of disease diagnosis and targeted therapies, and the mitigation of the industry's environmental impact.

Scientific Area:

Materials and technologies for Health and Environment

Quantum Materials and Quantum Technologies (Posters) / **117**

Effects of anisotropic correlations in fermionic zero-energy bound states of topological phases

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Topological phases of matter have been used as a fertile realm of intensive discussions about fermionic fractionalization. In this work, we study the effects of anisotropic superconducting correlations in the fermionic fractionalization on the topological phases. We consider a hybrid version of the SSH and Kitaev models with an anisotropic superconducting order parameter to investigate the unusual states with zero-energy that emerges in a finite chain. To obtain these zero-energy solutions, we built a chain with a well-defined domain wall at the middle of the chain. Our solutions indicate an interesting dynamic between the zero-energy state around the domain wall and the superconducting correlation parameters. Finally, we find that the presence of an isolated Majorana at the ends of the chain is strongly dependent on the existence of the solitonic excitation in the middle of the chain.

Quantum Materials and Quantum Technologies (Posters) / 118

Anisotropic scaling for 3D topological models

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A proposal to study topological models beyond the standard topological classification and that exhibit breakdown of Lorentz invariance is presented. The focus of the investigation relies on their anisotropic quantum critical behavior. We study anisotropic effects on three-dimensional (3D) topological models, computing their anisotropic correlation length critical exponent ν obtained from numerical calculations of the penetration length of the zero-energy surface states as a function of the distance to the topological quantum critical point. A generalized Weyl semimetal model with broken time-reversal symmetry is introduced and studied using a modified Dirac equation. An approach to characterize topological surface states in topological insulators when applied to Fermi arcs allows to capture the anisotropic critical exponent $\theta = \nu_x/\nu_z$. We also consider the Hopf insulator model, for which the study of the topological surface states yields unusual values for ν and for the dynamic critical exponent z. From an analysis of the energy dispersions, we propose a scaling relation $\nu_{\bar{\alpha}} z_{\bar{\alpha}} = 2q$ and $\theta = \nu_x/\nu_z = z_z/z_x$ for ν and z that only depends on the Hopf insulator Hamiltonian parameters p and q and the axis direction $\bar{\alpha}$. An anisotropic quantum hyperscaling relation is also obtained.

Materials and technologies for Health and Environment / 119

TBA

Advanced materials and processes for Energy / **120**

TBA

Quantum materials and quantum technogies / **121**

Quantum Materials and Quantum Technologies at CF-UM-UP

Author: Eduardo Castro[1]

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Initiated in 2014, CF-UM-UP is a joint effort comprising the Centro de Física da Universidade do Minho (CFUM) and the Centro de Física do Porto (CFP) to form a research centre in the broad area of Pure and Applied Physics. In this talk, examples of recent research on Quantum Materials and Quantum Technologies at CF-UM-UP will be presented. We will highlight collaborations with other research units from LaPMET as well as common research projects and recent joint activities.

Scientific Area:

Quantum materials and quantum technogies

New principles and technologies for sensing / **122**

Radiation Sensing using Superheated Liquids

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Our group fabricates and develops radiation detectors based on emulsions of superheated liquid droplets in a compatible gel matrix. The operation at reduced superheat renders the devices insensitive to minimum ionising particles that plague a variety of experiments aiming at the detection rare events induced by heavy/ier particles. The superheated emulsion is therefore an excellent tool for the detection of neutrons, alpha particles and heavy ions at low intensity levels. We will provide an overview of our application-oriented research activities in various areas: dark matter search for astrophysics, neutron dosimetry of massively shielded facilities, alpha detection for intrinsic soft error rate assessment in ultra-low activity nanoelectronic devices, alpha spectroscopy of contaminated liquid samples for emergency response and, more recently, colorimetric radiation sensing for radiation protection and public safety.

Scientific Area:

New principles and technologies for sensing

Advanced materials and processes for Energy / **124**

Advanced materials and processes for Energy @IFIMUP

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This presentation will give a brief overview of the research being performed at IFIMUP in the "Advanced materials and processes for Energy" research area.

Quantum materials and quantum technogies / 126

Manipulating hidden phases in Quantum Materials

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This talk aims at presenting the ongoing work in quantum materials, in progress at IFIMUP –LaPMET. After a short overview of the different ongoing research vectors, we will discuss two important examples involving static and dynamic excitations in order to stabilize hidden phases in non-equilibrium state, taking advantage of the strongly correlation between different excitations, the unconventional types of microscopic ordering and functional properties.
The recent E-FiELD project consists in strain-engineering strongly correlated perovskites to achieve an unprecedent electric-field control of electronic transport and optic properties, grounded on their cross-coupling between different degrees of freedom. We rely on recent theoretically developments that can enable the electric-field control of charge and orbital ordering, ferroelectricity, magnetism and metal-insulator phase transitions.
Finally, we will discuss how ultrafast coherent electromagnetic radiation at THz range can drive specific phonons in in complex oxide materials. In this regard, we will show how THz-driven polar phonons can be used to coherently manipulate macroscopic magnetic states, through a dynamical magnetoelectric coupling.

Scientific Area:

Quantum materials and quantum technogies / 127

Quantum Materials at C2TN

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Scientific Area:

Quantum materials and quantum technogies

Materials and technologies for Health and Environment / 128

Materials and Technologies for Health and Environment @ CF-UM-UP

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Materials and Technologies for Health and Environment @ CF-UM-UP

Scientific Area:

Materials and technologies for Health and Environment

New principles and technologies for sensing / **129**

New Principles and Technologies for Sensing @ FC-UM-UP

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New Principles and Technologies for Sensing @ FC-UM-UP

Scientific Area:

New principles and technologies for sensing

Materials and technologies for Health and Environment / **130**

Ultrashort laser pulses in Medical Imaging

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Ultrashort laser pulses deliver broadband sources for excitation of multiple fluorophores at the same time, therefore providing to medical imaging systems an advance tool for imaging deeper into samples. Furthermore, due to their short pulse duration, and smaller average power they also allow to extend the life time of in vivo samples. Ultrashort laser pulses can also be used in surgery for removing damaged tissues in very difficult areas with reduced access, therefore being excellent tools in medical applications.

New principles and technologies for sensing / **131**

NMR and sensing

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TBA

Scientific Area:

New principles and technologies for sensing

Materials and technologies for Health and Environment / 132

A multifunctional nano-approach for breast cancer therapy

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Breast cancer is the leading cause of cancer-related deaths in women worldwide [1]. The limitations of the current therapeutic highlight the need for new treatment modalities [2]. In this work, multifunctional lipid nanoparticles were developed for dual chemotherapy-photothermal therapy of breast cancer. Nanoparticles were also functionalized with different targeting agents to improve accumulation in breast cancer cells. Nanoparticles were optimized and fully characterized and demonstrated a high drug encapsulation efficiency and adequate properties for intravenous administration. A high anti-cancer efficacy was obtained in both 2D and 3D cell models of breast cancer [1]. Photothermal therapy was then explored by incorporating gold nanorods in the nanosystem. First, the influence of the NIR laser used (pulsed versus continuous) and other relevant parameters including the concentration of nanorods, the volume of the sample, and laser power settings were evaluated. Based on these results, the continuous laser was selected for further studies and an improvement of cancer cell death was obtained following laser irradiation after treatment with the developed nanoparticles. Finally, a preliminary *in vivo* biodistribution study was conducted in mice using IVIS® Optical Imaging.

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Quantum Materials and Quantum Technologies / 133

Quantum electrodynamics with polaritons in 2D materials

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Abstract: The description of several light-matter interaction phenomena at the nanoscale requires a quantum description of the electromagnetic field. This task is complicated when the electromagnetic field does not exist in a vacuum, but permeates a dielectric medium. In this case, the photons of the electromagnetic field couple to the dielectric degrees of freedom, giving origin to hybrid quasiparticles, which are referred to as polaritons. In order to describe polaritons, one must quantize the electromagnetic field in the presence of a dispersive material medium. However, the standard quantization approach does not work in the presence of dispersion. In this talk, we will describe a quantization approach that solves this issue. Our method allows us to, in principle, quantize polaritons in dispersive media with arbitrary geometry. The description of quantum polaritons in terms of modes allows to isolate the physical response of polaritons, from other radiative modes or lossy effects. In Ref. [1], we used the method to describe the decay rate of a quantum emitter due to graphene plasmon-polariton emission. Comparing the plasmon-polariton emission with the full decay rate, we conclude that, in certain conditions, the decay rate is dominated by emission of plasmons. We also used our quantization method to study the coupling of nitrogen-vacancy color centers mediated by exciton-polaritons hosted by two-dimensional transition metal dechalcogenides [2]. We find that by controlling the separation between two nitrogen-vacancy color centers, we can bring the emitters into the superradiant regime.

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Materials and technologies for Health and Environment / 134

Multifunctional nanocomposite membranes for environmental remediation of contaminants of emerging concern

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Human health and well-being strongly depend on water quality available for consumption. Deterioration of water quality has become one of the most worrying and urgent problems since about 1.6 million people die annually from illness related to unsafe water consumption, being responsible for at least 3900 children deaths per day in developing countries. In this scope, one of the main concerns is the release of emerging pollutants, such as pharmaceuticals and heavy metals, into wastewater [1].
Combining multifunctional membranes and photocatalytic, adsorbent, and antimicrobial materials in a unique membrane is considered one of the most suitable strategies for environmental remediation [1-2].
For this purpose, Ag-TiO2, Au-TiO2 and Y2(CO3)3 nanoparticles were synthesized and immobilized within poly(vinylidene fluoride-hexafluoropropylene), (PVDF-HFP). The physical-chemical properties of the fillers and membranes were characterization, together with the As(V) adsorption, and norfloxacin (NOR) photocatalytic removal efficiency, and antimicrobial activity.

The Y@Au-TiO2/PVDF-HFP multifunctional membranes present an efficiency of 89% in the degradation of NOR under ultraviolet (UV) radiation, 70% under visible radiation, and 93% in As(V) adsorption from water containing both contaminants simultaneously. The Ag-TiO2/PVDF-HFP multifunctional membranes show degradation efficiencies of 64.2% under UV and 80.7% under visible radiation, for 90 and 300 minutes, respectively. Furthermore, the recyclability of the multifunctional membranes has also been demonstrated. Finally, it was shown the antimicrobial activity of the nanocomposite membranes against E. coli and S. epidermidis.
In short, these results demonstrate the suitability of the produced nanocomposite membranes of Y@Au-TiO2/PVDF-HFP and Ag-TiO2/PVDF-HFP as multifunctional materials for environmental remediation.

Quantum Materials and Quantum Technologies / 135

Conducting bilayer salts (CNB-EDT-TTF)4A

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During the last few years a new paradigm of 2D conductors based on molecular bilayers, rather than on single layers, has emerged in a series of charge transfer salts based on the organic donor CNB-EDT-TTF (5-cyanobenzene-ethylenedithio-tetrathiafulvalene)[1], with different small anions A (I3–, ClO4–, BF4–, ReO4–, PF6–and SbF6–, AsF6–, AuI2–, I2Br–, etc⋯), with general formula (CNB-EDT-TTF)4A which has been reported by our group.[2-8] A common structural feature of this series of compounds is the head-to-head arrangement of the donors, induced by a network of weak C≡N⋯H–C interactions, which can be described as an effective combination of R22(10) and R24(10) synthons, forming donor bilayers alternating with anionic layers. This series of layered compounds is characterized by a so far unique arrangement of partially oxidized donors in bilayers with interesting two-dimensional metallic or even superconducting properties. They present a rich diversity of polymorphs with different origins: i) different layer packing patterns of donors; ii) alternating or uniform arrangement of donors tilting between successive bilayers; iii) distinct anionic lattices and possible anion ordering schemes. The contribution of the different possible anion layer and interlayer ordering schemes to the structural variations observed will be presented together with their physical properties.

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