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MAP-fis Conference 2016

Physics Department Auditorium, University of Aveiro

July 1st, 2016

PD F PROGRAMAS DE DOUTORAMENTO FCT

CONFERENCE PROGRAM

09:00	**Opening**		
09:15	A1	Ana Rita da Silva Rocha Frias	Enhancement of photovoltaic energy conversion by downshifting with organic-inorganic hybrids
09:30	A2	Vivian Maria Campos Soares de Andrade	Synthesis of (GdTb)/FeCo)2 compounds for magnetostrictive and magnetocaloric studies.
09:45	A3	Bernardo Daniel Antunes Bordalo	Thermal Switches in Solid State Magnetic Refrigeration: Conductivity Change Requirements and Effects
10:00	A4	Cesar Rui de Freitas Bernardo	CINÉTICA DE DECAIMENTO FOTOLUMINESCENTE EM FILMES FINOS DE PONTOS QUÂNTICOS.
10:15	A5	Pedro Rafael dos Santos Prezas	TSDC MEASUREMENTS ON Ca10(PO4)6(OH)2 Beta-Ca3(PO4)2 AND BIPHASIC BIOCERAMICS
10:30	A6	Bogdan Postolnyi	DEPOSITION AND STUDY OF MULTILAYER COATINGS BASED ON METAL NITRIDES
Coffee Break			
11:15	B1	Nuno Miguel Azevedo Silva	LOCAL MANAGEMENT OF THE NONLINEARITY IN BOSE EINSTEIN CONDENSATES
11:30	B2	Hugo Manuel Castro Gonçalves	Macroscopic SHG induced at the surface of pNA nanocrystals embedded in polymeric nano-fiber scaffolds.
11:45	B3	Cláudio Filipe Vieira Gomes	Scalar field inflation in the presence of a non-minimal matter-curvature coupling
12:00	B4	Catarina Cosme	Scalar field dark matter and the Higgs field
Lunch and Posters			
15:15	C1	Sangeetha Balabhadra	LANTHANIDE ION LUMINESCENCE AS A TOOL FOR NANOTHERMOMETRY
15:30	C2	Ana Rita Oliveira Rodrigues	LIPOSOMES ENTRAPPING MnFe2O4 NANOPARTICLES AS NANOCARRIERS FOR ANTITUMOR DRUGS
15:45	C3	Carlos de Oliveira Amorim	UTILIZATION OF PAC OF RADIOISOTOPE TRACKERS AND DFT CALCULATIONS TO DETERMINE LOCAL ENVIRONMENT OF Hg(II) IN DITHIOCARBAMATE FUNCTIONALIZED PARTICLES FOR MAGNETIC REMOVAL OF Hg2+ FROM WATER
16:00	C4	Guilherme Domingos Carvalho Teixeira	Variability study of the high-resolution spectra of an O-star - Preliminary findings
Coffee Break			
16:45	D1	Rui Miguel Abreu Vilarinho da Silva	Interplay of Structural Distortions and Physical Properties on Perovskites
17:00	D2	Niaz Ali Khan	THE KERNEL POLYNOMIAL SIMULATION OF QUANTUM SYSTEMS
17:15	D3	Anselmo Miguel Magalhães Marques	Edge currents in frustrated Josephson junction ladders
17:30	D4	Miguel Noronha da Canhota	INTENSE ULTRASHORT LASER PULSES BY MULTI-PLATE CONTINUUM GENERATION
17:45	D5	Ana Rita Ribeiro	OPTICAL FIBERS FOR BEAM SHAPING AND TRAPPING

Poster Session			
14:00:15:15	P1	Icaro Jael Mendonça Moura	Structural and Electronic Properties Calculations of Two-dimensional Materials
	P2	Jennifer Cláudia Passos Teixeira	INFLUENCE OF CdS AND ZnxSn1-xOy BUFFER LAYERS ON THE PHOTOLUMINESCENCE OF Cu(In
	P3	Sandra Filipa Henriques Correia	Scale up the collection area of luminescent solar concentrators towards metre-length flexible waveguiding photovoltaics
	P4	Sílvia Maria Gouveia Rodrigues	Modelling and simulation of nonlinear optical phenomena in hollow-core photonic crystal fibres
	P5	Catarina Dias	MgO as a Resistive Switching Layer
	P6	Alexandre Manuel Pedroso Botas	CHANGES ON THE LIGHT EMISSION FEATURES OF CRYSTALLINE SILICON NANOPARTICLES INDUCED BY SURFACE MODIFICATION
	P7	Helgi Freyr Rúnarsson	Kerr black holes with hair: shadows
	P8	André Gomes da Costa Guerra	Ocean Monitoring with Small Satellites

A1 – ENHANCEMENT OF PHOTOVOLTAIC ENERGY CONVERSION BY DOWNSHIFTING WITH ORGANIC-INORGANIC HYBRIDS

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Organic-inorganic hybrids are promising candidates for a wide range of applications like fuel cells, optics, photonics, microelectronics and others [1]. However, their application as downshifting materials for photovoltaic (PV) cells has not yet been widely explored. The application of down-shifting layers have been proposed as a method to improve the spectral response of solar cells to short-wavelength radiation. For example, the most used PV cells are Si-based with low performance for ultraviolet photons. The incorporation of organic-inorganic down-shifting layers in PV modules can provide a cheap and effective way to integrate photons conversion [3]. Down-converting layers can be seen as distinct type of cost-effective devices easily integrated in PV energy conversion. Moreover, these devices can promote the integration of PV architectural elements into buildings, with the unprecedented possibilities for energy harvesting in façade design, urban furnishings and wearable solar fabrics. In this work, organic-inorganic hybrid (named as tri-ureasil) doped with organic dyes (e.g. rhodamine 6G, rhodamine 800 and silicon 2,3-naphthalocyanine bis(trihexylsilyloxide)) will be used as down-shifting layers and the external quantum efficiency of Si PV cells will be evaluated.

[1] C. Sanchez, K. J. Shea, S. Kitagawa, and K. J. Sanchez Clément, "Applications of advanced hybrid organic–inorganic nanomaterials: from laboratory to market," *Chem. Soc. Rev.*, vol. 40, no. 2, pp. 588–595, 2011.

[2] S. F. H. Correia, V. De Zea Bermudez, S. J. L. Ribeiro, P. S. André, R. a S. Ferreira, and L. D. Carlos, "Luminescent solar concentrators: Challenges for lanthanide-based organic-inorganic hybrid materials," *J. Mater. Chem. A*, vol. 2, no. 16, pp. 5580–5596, 2014.

[3] T. Fix, A. Nonat, D. Imbert, S. Di Pietro, M. Mazzanti, A. Slaoui, and L. J. Charbonnière, "Enhancement of silicon solar cells by downshifting with Eu and Tb coordination complexes," *Prog. Photovolt Res. Appl.*, vol. 15, pp. 659–676, 2016.

A2 – SYNTHESIS OF (GD,TB)(FE,CO)2, COMPOUNDS FOR MAGNETOSTRICTIVE AND MAGNETOCALORIC STUDIES.

Vivian Maria Campos Soares de Andrade

A3 - THERMAL SWITCHES IN SOLID STATE MAGNETIC REFRIGERATION: CONDUCTIVITY CHANGE REQUIREMENTS AND EFFECTS

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Typical magnetocaloric refrigerators use an alternated fluid flow to drive the heat from the cold to the hot reservoir, which limits both their size and efficiency. [1] A solid state magnetic refrigerator trades the traditional fluid flow to control the heat flux in an active magnetic regenerator by two solid thermal switches (TSs). These TSs have an externally controllable thermal conductivity (k), which can be changed to $k \pm \Delta k$ to in effect allow (+) or block (−) the passage of heat through the TS. By using two TSs in synchrony with the magnetocaloric effect in a Brayton cycle for refrigeration one can choose to have most of the heat flux from the magnetocaloric material (MCM) to the hot reservoir when under an applied magnetic field, and to have most of the heat absorbed by the MCM come from the cold reservoir when that field is removed.
Previous work assumed ideal TSs, [2] which have null k in the OFF state. Here we investigate the required conductivity change between the ON and OFF states (Δk) and the effects this change has under different working temperatures (T_0) and frequencies (f). We tested three different materials, with approximately an order of magnitude of difference in their k values, 401 W/(m K), 18 W/(m K) and 1.6 W/(m K). Results show the gain in temperature difference between the hot and cold reservoirs as a function of different operating conditions Although the active magnetic regenerator already imposes a temperature difference between the two reservoirs under most conditions, the use of thermal switches with a $\Delta k \approx 70$ % can add 1 K to the temperature difference with the lowest k TSs.

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A4 -CINÉTICA DE DECAIMENTO FOTOLUMINESCENTE EM FILMES FINOS DE PONTOS QUÂNTICOS.

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Os pontos quânticos (QDs) são promissores blocos de construção luminescentes para uma extensa gama de aplicações [1]. Para um bom aproveitamento destas nanoestruturas é necessário um conhecimento profundo da sua dinâmica de fotoluminescência.[2]

Neste trabalho apresentamos um estudo da cinética de decaimento entre os QDs incorporados em matrizes poliméricas utilizando sistemas de iluminação epi-fluorescente [3] e reflexão total interna. Os dados experimentais foram analisados usando um modelo que não requer conhecimento prévio da distribuição (exponenciais) e modelos que correspondem as distribuições pré-assumidas (stretched exponential, gamma) [4]. Sendo que a soma de gammas permite obter o máximo de informação física relevante.

[1] A. L. Rogach (ed.), Semiconductor Nanocrystal Quantum Dots, Springer-Verlag: Wien (2008).

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A5 - TSDC MEASUREMENTS ON $Ca_{10}(PO_4)_6(OH)_2$, -$Ca_3(PO_4)_2$ AND BIPHASIC BIOCERAMICS

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Synthetic Hydroxyapatite [Hap, $Ca_{10}(PO_4)_6(OH)_2$] based bioceramics have been highlighted over the last four decades due to their structural and compositional analogousness with the biologic Hap [1,2], i.e., the one which occurs naturally in our organism and is the main component of bones (65 to 70 wt%). These biomaterials display bioactivity and osteoconductivity processes [2]. However, the rate at which Hap-based bioceramics promote the growth of new host bone, which is related with the osteoconductivity and resorption/dissolution processes, is still considered unsatisfactory. Among the methods being researched to enhance host bone formation, the electrical polarization of these materials is the one with the most remarkable results, accelerating considerably the host bone growth [3]. The electrical polarization of beta-tricalcium phosphate [β-TCP, β-$Ca_3(PO_4)_2$] bioceramics is a recent subject, with the first publications dating back to 2010. Curiously, some of the first publications are contradictory: in reference [4], for instance, it is stated that β-TCP is not polarizable, while in [5] it is stated that β-TCP has a suitable composition and structure for ion conduction and a large electrical charge storage ability.

In the present work the electrical polarization of pure Hap and β-TCP, and biphasic (75Hap-25β-TCP wt%) bioceramics was analyzed by measuring thermally stimulated depolarization currents (TSDC). The samples were thermo-electrical polarized at temperatures between 250 and 500 ºC. At such temperatures, with external electrical field amplitudes in the order of 1-5 kV/cm, the ionic mobility is activated, enabling stored charge densities in the order of 10^{-8}-10^{-2} C/cm^2 to be achieved. From the TSDC spectra, the total stored charge density for a given polarization temperature and the activation energy of each depolarization process were calculated.

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[5] W. Wang, S. Itoh, N. Yamamoto, A. Okawa, A. Nagai, K. Yamashita, *Electrical polarization of β-Tricalcium phosphate ceramics*, Journal of the American Ceramic Society, 93(8) 2175-2177 (2010)

A6 - DEPOSITION AND STUDY OF MULTILAYER COATINGS BASED ON METAL NITRIDES

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Over the last decades the class of transition metal coatings is under the focus of material science and the interest in such kind of materials is still growing. They have plenty of applications and functional proposes, but most of them can be characterized by good mechanical properties which allows using of metal nitrides as protective and decorative coatings. The main task is to exist deposition conditions to obtain materials with predicted properties.
It was observed that a grains size may cause changes of mechanical properties of thin films, e. g. increasing grains diameter to nanoscale dimensions sometimes increases values of hardness. Other approach to change mechanical properties is design of multilayer structures in coatings. Both methods increase interface volume in films and can be controlled during films deposition.
This research is devoted to deposition and study of a few sets of metal nitride coatings fabricated in single layer and multilayer states. Films based on Titanium, Molybdenum, Chromium, Aluminium nitrides were obtained by cathodic arc deposition and magnetron sputtering. Their elemental-phase composition and structure, as well as some mechanical properties, were measured by various techniques. The dependence of structure and properties on deposition conditions, layer thickness and grain size was observed.

B1 - LOCAL MANAGEMENT OF THE NONLINEARITY IN BOSE EINSTEIN CONDENSATES

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Spatiotemporal management of nonlinearities is emerging as a new tool for the manipulation of soliton dynamics[1]. In particular, for the case of matter-wave solitons of Bose Einstein Condensates, these so called “collisionally inhomogeneous media” has been a playground for novel nonlinear phenomena, which include adiabatic compression of matter waves[2], atomic soliton lasers and interferometers[3], enhanced transmission of matter-waves through a potential barrier[4], observation and control of Faraday waves[5] and Bloch oscillations and dynamical trapping of matter wave solitons[6]. Unfortunately for many interesting experiments involving spatial varying nonlinearities, the standard approach of the Feshbach resonance management has proven to be unsuitable due either to length scale mismatches or additional parasitic effects[7,8]. Here we explore the possibility of controlling the inhomogeneities in quasi-1D Bose Einstein condensates using a spatial variation of the transverse confinement potential[9] and present some early stage results on the dynamics of matter-wave solitons in such systems using computational simulations of the full 3D Gross-Pittaevski equation.

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B2 - MACROSCOPIC SHG INDUCED AT THE SURFACE OF *P*NA NANOCRYSTALS EMBEDDED IN POLYMERIC NANO-FIBER SCAFFOLDS.

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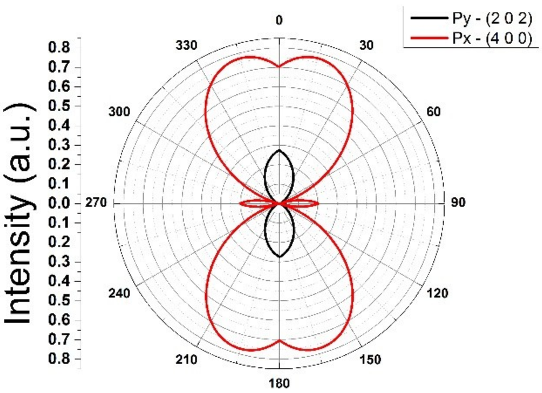
Quadratic nonlinear optical phenomena are forbidden in centrosymmetric media, within the dipole approximation. However, a medium that is centrosymmetric in the bulk necessarily loses that symmetry at its surface. The theoretical work done by Munn and his co-workers quantified the surface induced SHG in a crystal of *p*-nitroaniline (*p*NA)[1,2].

In this study the theoretical approach of Munn, for the SHG at the surface of *p*NA crystal, is used to detail the polarization dependence analysis in a set of polymeric nanofibers doped with *p*NA[3,4]. The polymeric nanofibers are used as scaffolds where the organic chromophores are arranged into suitable organizations for generating NLO effects, in particular to promote second order NLO effects. These supramolecular systems are fabricated on a 1D sub-wavelength scale by electro-spinning techniques where the strong electric field, used in the deposition, forces the alignment of the organic material to add up constructively. The manipulation of the parameters and the choice of the polymeric matrix host can be optimized to obtain the best orientation plan to induce SHG.

Polarimetry analysis demonstrates well-oriented dipole moments inside the nanostructure, while the spectrum of the SHG is wide-band indicating the extreme thinness of the active sections. X-Ray analysis and the analytical data fit, according to Munn approach, were used as tools to reveal the symmetry plane that induces macroscopic SHG.



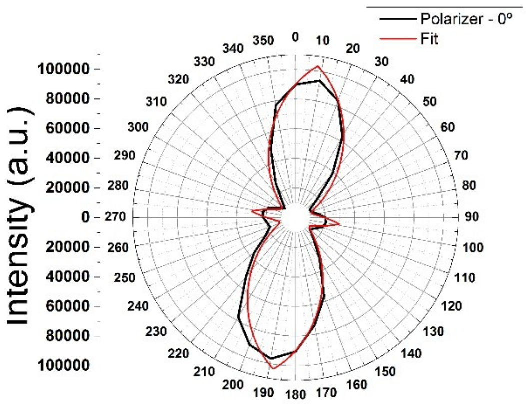


Figure 1 – (Left) Theoretical response of SHG induced by a plane orientation (4 0 0) and (2 0 2) in a crystal surface of *p*NA using the theory of Munn. (Right) Experimental data of a PMMA nanofibers doped with *p*NA and the respective fit using the theoretical expression of Munn for the plane orientation (2 0 2). The orientation was confirmed by X-ray analysis.

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[2] – Munn, R. W. J. Chem. Phys. 1992, 97 (6), 4532.
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B3 - SCALAR FIELD INFLATION IN THE PRESENCE OF A NON-MINIMAL MATTER-CURVATURE COUPLING

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We study the non-minimal matter-curvature coupling effects in inflation driven by a scalar field. We obtain a modified Friedmann equation that in the high density regime yields different inflationary behaviour when compared with usual General Relativity's one. Compatibility with Planck's data is examined.

[1] O. Bertolami, C. Gomes, J. Rosa, in preparation...

B4 - SCALAR FIELD DARK MATTER AND THE HIGGS FIELD

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We discuss the possibility that dark matter corresponds to an oscillating scalar field coupled to the Higgs boson. We argue that the initial field amplitude should generically be of the order of the Hubble parameter during inflation, as a result of its quasi-de Sitter fluctuations. This implies that such a field may account for the present dark matter abundance for masses in the range $10^-6 - 10^-4$ eV, if the tensor-to-scalar ratio is within the range of planned CMB experiments. We show that such mass values can naturally be obtained through either Planck-suppressed non-renormalizable interactions with the Higgs boson or, alternatively, through renormalizable interactions within the Randall-Sundrum scenario, where the dark matter scalar resides in the bulk of the warped extra-dimension and the Higgs is confined to the infra-red brane.

C1 - LANTHANIDE ION LUMINESCENCE AS A TOOL FOR NANOTHERMOMETRY

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Non-contact temperature measurements with accurate high spacial and degree resolution became imperative and creates a need to develop new techniques to meet these requirements. At this front, temperature dependent lanthanide ion luminescence begin to be a promising tool for thermal sensing applications in microelectronics, nanotechnology and nanomedicine [1,2]. Luminescent nanothermometers doped with Yb^{3+}/Er^{3+} (upconversion) and Nd^{3+} (downshifting) embedded into different host matrices like Gd_2O_3 and SrF_2 were studied for thermometry [3,4]. The change in the temperature on their luminescence is calculated through the fluorescence intensity ratio (FIR) method. Furthermore, the performance of the developed nanothermometers is calculated in the form of their Sensitivity.

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C2 - LIPOSOMES ENTRAPPING $MnFe_2O_4$ NANOPARTICLES AS NANOCARRIERS FOR ANTITUMOR DRUGS

Ana Rita O. Rodrigues,[1] I. T. Gomes,[1,2] Bernardo G. Almeida,[1] J. P. Araújo,[2] Maria João R. P. Queiroz,[3] Paulo J. G. Coutinho,[1] Elisabete M. S. Castanheira[1]

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Liposomes entrapping magnetic nanoparticles (magnetoliposomes) are advantageous therapeutic systems as they can overcome many pharmacokinetics problems and can be guided and localized to the sites of interest [1,2]. The use of magnetoliposomes as nanocarriers allows a safer use of powerful drugs with lower drug dosage and a more efficient treatment.

In this work, manganese ferrite nanoparticles (NPs), with size distribution of 26±7 nm, and superparamagnetic behavior at room temperature (Fig. 1A), were synthesized [3]. These NPs were either entrapped in liposomes, originating aqueous magnetoliposomes (AMLs), or covered with a lipid bilayer, forming solid magnetoliposomes (SMLs).The latter were prepared by a new method developed by us [4]. Membrane fusion between AMLs (Fig. 1B) and SMLs with giant unilamellar vesicles (GUVs), used as membrane models was confirmed by FRET assays. For that, the labeled lipid NBD-C_{12}-HPC and the hydrophobic dye Nile Red (or the labeled lipid Rhodamine B-DOPE) were both incorporated in the lipid bilayer of magnetoliposomes, the NBD moiety acting as the energy donor and the dye Nile Red (or Rhodamine B) as the energy acceptor. Keeping in mind future drug delivery applications, both AMLs and SMLs were tested as nanocarriers for a new promising antitumor drug, a thienopyridine derivative [3].

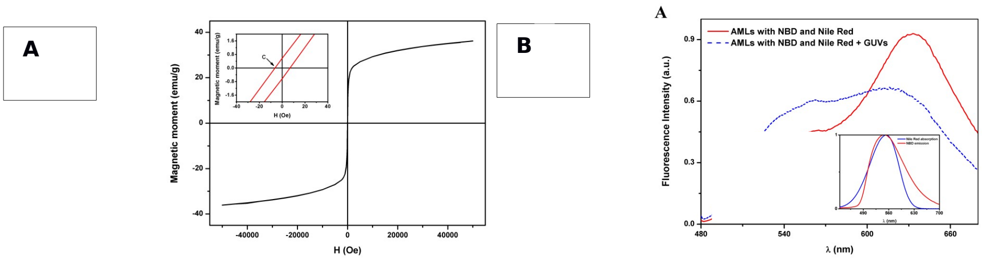

Figure 1 A. Magnetization hysteresis loop of $MnFe_2O_4$ NPs measured at room temperature. Inset: Enlargement of the loop, in the low field region. **B.** Fluorescence spectra (λ_{exc}=400 nm) of AMLs containing both NBD-C_{12}-HPC and Nile Red, before and after interaction with GUVs.

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C3 - UTILIZATION OF PAC OF RADIOISOTOPE TRACKERS AND DFT CALCULATIONS TO DETERMINE LOCAL ENVIRONMENT OF Hg(II) IN DITHIOCARBAMATE FUNCTIONALIZED PARTICLES FOR MAGNETIC REMOVAL OF Hg2+ FROM WATER

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The application of nanoparticles in water treatment technology has attracted growing interest due to their high specific surface area and ability for surface chemical functionalization. In particular, functionalized iron oxide nanoparticles have been very promising sorbents because several pollutants can be adsorbed and then removed from the solution resorting to the application of an external magnetic field [1-2].

It has been reported a new strategy for the surface modification of magnetite particles that resulted into magnetic sorbents with silica shells enriched in dithiocarbamate groups, with the finality of removing heavy metals from water (in particular the highly toxic mercury) [3-4].

The importance of dithiocarbamate groups for an effective Hg(II) uptake as well as operational parameters (such as sorbent dose, initial Hg concentration, equilibration time, and pH) have already been studied, however the chemical mechanism behind the adsorption of all the possible nanoparticles are currently unknown.

Using Perturbed Angular Correlations (PAC) Spectroscopy [5] of 199Hg radioisotope we were able to identify different local environments that characterize the position where the Hg is retained during the adsorption. These local environments and their specific electric field gradients (EFG) were than compared with theoretical scenarios and respective DFT calculations (LDA and GGA-PBE calculations).

This crossover between PAC experimental data analysis and DFT calculations allow us to infer the mechanism which gives rise to the absorption of the different nanoparticle functionalizations.

We also present an alternative method to determine the adhesion/uptake of the Hg(II) by the different types of nanoparticles, resorting to direct tracking of tracking of the radioisotope. This method shows many advantages when comparing with indirect quantification since it requires much less mass of analyzed sample and allows us to study directly what happens to the Hg(II) when the Nanoparticles are manipulated prior to the Hg uptake. This paves the way to studies regarding the nanoparticles recycling and manipulation conditions as well as studies of the path taken by heavy metals in flora and fauna

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C4 - VARIABILITY STUDY OF THE HIGH-RESOLUTION SPECTRA OF AN O-STAR

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Abstract:
Massive O-stars are some of the most enigmatic astronomical stellar objects. Their masses have significant impact in the overall physics of their atmospheres.
We have performed a study of the variability in the spectra of an O-star using high-resolution spectroscopic observations.
I will present some of our preliminary findings and discuss some of their implications on our understanding of the physical processes driving these stars.

D1 - INTERPLAY OF STRUCTURAL DISTORTIONS AND PHYSICAL PROPERTIES ON PEROVSKITES

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The demand for new materials with higher performance and versatility has been focused on those exhibiting coupling between elementary excitations [1]. The transition metal oxides with perovskite structure (AMO_3, A = large ion, M = transition metal), have been largely studied, as these materials exhibit strong coupling between orbital, electronic, spin and lattice degrees of freedom [1]. Among them, rare-earth oxides (RMO_3, R = rare-earth) offer different ways of tuning their structural and physical properties, which has deserved much attention from both theoretical and experimental point of views.
Our work aims at studying the physical properties of some promising materials ($RMnO_3$, $RFeO_3$, and the solid solution $TbMn_{1-x}Fe_xO_3$) and to disentangle how they are associated with the type of crystallographic structure. The main goals are to ascertain the evolution of the important MO_6 octahedra distortions, their tilting and Jahn-Teller deformation, focusing on their correlation with the electronic and magnetic interactions, via spin-phonon coupling, which will ultimately determine their physical properties. We will show how in the chosen compounds, the aforementioned mechanisms can be highlighted through a structural study as a function of the rare-earth ion (r_R) and substitution ratio [2-3]. Moreover, different external parameters such as temperature, magnetic field and hydrostatic pressure can be used to allow a deeper understanding of the interplay between structural and physical properties [4-5]. The main outcomes of our study will enable a better insight onto the role of those structural distortions on the stabilization of magnetic structures and their effect on the physical properties.

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D2 - THE KERNEL POLYNOMIAL SIMULATION OF QUANTUM SYSTEMS

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Abstract:

The investigation of the quantum properties of matter in condensed-matter physics is a difficult task, especially for a large systems with whose models are too complex to allow for analytical solutions. Therefore numerical simulations are required to examine the nature of such quantum systems.

In comparison with other numerical methods, the kernel polynomial method (KPM)[1,2] is one of the most efficient and competitive numerical techniques to calculate properties of the very large Hamiltonians important in computational materials science. It is based on the Chebyshev polynomial expansion of a function. The Chebyshev expansion allows a very precise calculation of the spectral properties of large sparse matrices [3].

In this review, we describe the kernel polynomial methods (KPM) estimates for densities-of-states (DOS) also known as spectral density, local densities-of-states (LDOS) and correlation functions of one-electron Hamiltonians with and without disorder. The KPM method enables us to efficiently calculate DOS or LDOS without the need to exactly diagonalize the Hamiltonian. The method is demonstrated for tight binding models for both pure and disordered systems [1-4].

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D3 - EDGE CURRENTS IN FRUSTRATED JOSEPHSON JUNCTION LADDERS

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We present a numerical study of quasi-1D frustrated Josephson junction ladders with diagonal couplings and open boundary conditions, in the large capacitance limit [1]. We derive a correspondence between the energy of this Josephson junction ladder and the expectation value of the Hamiltonian of an analogous tight-binding model [2], and show how the overall superconducting state of the chain is equivalent to the minimum energy state of the tight-binding model in the subspace of one-particle states with uniform density. To satisfy the constraint of uniform density, the superconducting state of the ladder is written as a linear combination of the allowed k-states of the tight-binding model with open boundaries. Above a critical value of the parameter t (ratio between the intra-rung and inter-rung Josephson couplings), the ladder spontaneously develop currents at the edges which spread to the bulk as t is increased until complete coverage is reached. Above a certain value of t, which varies with ladder size (t = 1 for an infinite-sized ladder), the edge currents are destroyed. The value t = 1 corresponds, in the tight-binding model, to the opening of a gap between two bands. We argue that the disappearance of the edge currents with this gap opening is not coincidental, and that this points to a topological origin for these edge current states.

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D4 - INTENSE ULTRASHORT LASER PULSES BY MULTI-PLATE CONTINUUM GENERATION

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Multi-plate continuum (MPC) [1] is a new solid-state-based spectral broadening process for the generation of high-energy ultrashort pulses that avoids common pitfalls from regular spectral broadening in bulk materials, such as low damage threshold and low input/output energy.
In this work, we focused an infrared laser pulse (sub-30 fs in duration) from our ultrafast laser amplifier into a set of thin (100 μm) fused silica plates, spatially separated from each other, and positioned within the Rayleigh range of the beam. The beam arising from the plates is spectrally broadened and spatially very homogeneous, which potentially leads to shorter pulses compared with the initial input pulse.
We present a temporal characterization of the ultrashort pulses created by MPC, using the dispersion scan (d-scan) technique [2], which evidences that we are able to create sub-13 fs pulses with high efficiency. These shorter pulses can be directly employed for important applications such as high-resolution ultrafast spectroscopy and high-harmonic generation experiments, while being much easier to use when compared to other alternatives such as gas-filled hollow-core fibers (HCFs).

Figure 0: Spectrum and spectral phase of the impulse

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D5 - OPTICAL FIBERS FOR BEAM SHAPING AND TRAPPING

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Beams carrying optical momentum, such as optical vortices, have been employed in a large myriad of fields, from optical trapping and rotation of particles, to quantum communications, among others. Typically, the techniques used to generate OVs are based on free space bulk setups, using diffractive gratings, via spatial light modulators or specially designed optical components, such as cylindrical or spiral phase plates. So far, few and still too complex possibilities have been described, concerning the generation of such beams, using miniaturized platforms such as optical fibers. Ultimately, these prototypes of spiral phase lenses unveil new possibilities in the miniaturization and possible integration into optofluidic platforms.
In this talk, a method for the generation of optical vortices based on micropatterned optical fiber tips will be presented. The spiral phase plates are micro machined on the tip of optical fibers using a focused ion beam. The plate act as a beam tailoring system, transforming the fundamental guided mode, specifically a Gaussian mode, into the Laguerre-Gauss mode, carrying orbital angular momentum. Insights on the modulation, fabrication, experimental results and further application as an optical tweezers system will be addressed. Besides this, other structures suitable for optical trapping will be briefly mentioned.

P1 - STRUCTURAL AND ELECTRONIC PROPERTIES CALCULATIONS OF TWO-DIMENSIONAL MATERIALS

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When graphene was first isolated in 2004, a great research interest begun and has since been growing. Graphene shows unique properties that can be exploited both in fundamental research and in technological applications. Other two dimensional (2D) materials like hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDC) have equally interesting properties giving rise to the research area of 2D materials which is exponentially growing [1]. Based on first principle calculations made with the Density Functional Theory (DFT) package QUANTUM ESPRESSO [2] , we present structure calculation results for the following 2D materials: graphene, hBN and MX_2 (M = W, Mo; X = S, Se). These calculations were made using nonrelativistic (NR) and full relativistic (FR) pseudopotentials (PP) with the PBE exchange-correlation functional [3]. NR calculations were made with a linear spin polarization without spin-orbit (SO) interactions whereas FR calculations were made with non-collinear spin polarization with SO. In comparison with the known experimental values, the results for lattice constant are accurate to 0.5% for graphene, 1.0% for hBN and 1.9-2.7\% for TMD. Band structure calculations revealed the known results that graphene is a semimetal with no bandgap, hBN is insulating with an indirect bandgap, and all 2D TMD have direct bandgaps at the K point. All bandgap values for hBN and TMD obtained are in good agreement with the results of DFT simulations reported in the literature [4] These results show that two-dimensional materials structural and electronic properties can be accurately determined by DFT calculations and promote confidence for more interesting calculations.

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Support by CAPES, MEC, BRAZIL, PhD grant is gratefully acknowledged.

This work was supported by the Portuguese Foundation for Science and Technology (FCT) in the framework of the Strategic Funding UID/FIS/04650/2013.

P2 - INFLUENCE OF CdS AND $Zn_xSn_{1-x}O_y$ BUFFER LAYERS ON THE PHOTOLUMINESCENCE OF $Cu(In,Ga)Se_2$ THIN FILMS

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Thin film solar cells based on $Cu(In,Ga)Se_2$ (CIGS) have recently achieved an impressive world record of light to power conversion efficiency, 22.3 %[1]. This achievement has followed a number of developments based on improving the CIGS surface by a potassium post deposition method. Despite the scarce information available from Solar Frontier [1], ZSW achieved similar values of power conversion efficiency: 21.7 % for CdS-based devices and 21% for Cd-free based devices [2]. These improvements together with the need to replace the toxic CdS layer in the CIGS solar cell architecture, emphasize the necessity to study the CIGS/buffer layer interface and to fully understand its potential. The ideal buffer layer should have: i) better electrical properties than CdS, ii) non-toxic elements, iv) high bandgap energy, v) allow for a deposition by a vacuum compatible technique, and vi) be thinner than the current 50 nm thickness of the CdS layer [3]. In this work, we address this issue by using photoluminescence (PL) as a probing tool for the defects on CIGS and CIGS/buffer layer interface for two samples with different buffer layers, CdS and ZnSnO. A strong influence of fluctuating potentials [4] was observed for the samples with CdS and ZnSnO. A similar non-radiative de-excitation channel was obtained for both samples, despite the likely different density of charged defects. The study showed a reduction of electrostatic fluctuating potentials in the CIGS/ZnSnO sample in comparison with the CIGS/CdS one, showing that the ZnSnO semiconductor is a promising buffer layer for CIGS based solar cells and that the choice of the buffer layer also changes some of the properties of the CIGS absorber. This conclusion should be kept in mind when designing buffer layer materials and/or its deposition systems.

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P3 - SCALE UP THE COLLECTION AREA OF LUMINESCENT SOLAR CONCENTRATORS TOWARDS METRE-LENGTH FLEXIBLE WAVEGUIDING PHOTOVOLTAICS

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Luminescent solar concentrators (LSCs) are cost-effective components easily integrated in photovoltaics (PV) that can enhance solar cells' performance and promote the integration of PV architectural elements into buildings, urban furnishing and wearable fabrics. The devices' performance is dominated by the concentration factor (*F*), which is higher in cylindrical LSCs compared with planar ones (with equivalent collection area and volume)[1]. We use a drawing optical fibres facility to easily fabricate large-area LSCs (length up to 2.5 m) based on bulk and hollow-core plastic optical fibres (POFs)[2]. The active layers used to coat the bulk fibres or fill the hollow-core ones are Rhodamine 6G- or Eu^{3+}-doped organic–inorganic hybrids. For bulk-coated LSCs, light propagation occurs essentially at the POFs, whereas for hollow-core devices light is also guided within the hybrid. The lower POFs' attenuation (~0.1 m^{-1}) enables light propagation in the total fibre length (2.5 m) for bulk-coated LSCs with maximum optical conversion efficiency (η_{opt}) and F of 0.6% and 6.5, respectively. For hollow-core LSCs, light propagation is confined to shorter distances ($6–9\times10^{-2}$ m) because of the hybrids' attenuation (1–15 m^{-1}). The hollow-core optimized device displays η_{opt} = 72.4% and F = 12.3. The F values are larger than the best ones reported in the literature for large-area LSCs (F = 4.4)[3], illustrating the potential of this approach.

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P4 - MODELLING AND SIMULATION OF NONLINEAR OPTICAL PHENOMENA IN HOLLOW-CORE PHOTONIC CRYSTAL FIBRES

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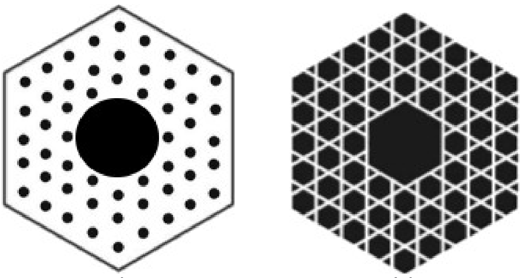
The hollow-core photonic crystal fibres (HC-PCFs) can guide light in different conditions, based on the photonic band gap effect [1-2]. Due to its periodic structure, the light is forbidden to propagate through the fibre's cladding and therefore it remains confined in the fibre's core. In practice, the core can be filled with the desired material: solid, liquid, gas, or plasma.

We present the main light guidance mechanisms that occur in HC-PCFs (fig. 1). In particular, we will analyse the kagomé fibres. We show some fibre's fundamental propagation modes obtained by computational methods. In addition, we present the nonlinear and dispersive properties of some HC-PCFs, and light propagation results showing the generation of supercontinuum and of UV light.



a) b)

fig. 1 - the geometry of some hollow-core MOFs: a) hexagonal fibre; b) kagomé fibre.

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P5 - MgO AS A RESISTIVE SWITCHING LAYER

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The development of conventional non-volatile memories is coming to a halt and novel approaches are being intensively pursued. The recent realization of memristors [1], nanodevices exhibiting non-volatile resistive switching, could be crucial in this endeavor, when used as Resistive Random Access Memories (ReRAMs) [2]. These can be fabricated in a simple structure allowing high-density implementation, have low-power operation as well as fast switching and large retention times [3]. On the other hand, MgO is a binary metal oxide with a high dielectric constant, band gap, thermal conductivity and breakdown field. Therefore, besides its importance in magnetic tunnel junctions, it is a highly attractive insulating material for ReRAMs [4].
In this work we present a thorough study on nonvolatile resistive switching in MgO-based metal-insulator-metal nanostructures. We successful achieved structures displaying large ON/OFF ratios (>10^4), endurance (>10^3 cycles) and retention (10^4 s) in a simple, high yield process (>90%). By varying the MgO thickness (from 15 to 40 nm) we could see clear increasing trends in the forming, reset and set voltages. These results can be explained using the numerically implemented random circuit breaker model.

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P6 - CHANGES ON THE LIGHT EMISSION FEATURES OF CRYSTALLINE SILICON NANOPARTICLES INDUCED BY SURFACE MODIFICATION

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Crystalline silicon nanoparticles (SiNPs) are a very promising material due to their unique properties, such as tunable and efficient luminescence [1, 2], which make them attractive for application in fields as bioimaging [3] or light emitting devices [4]. To enable a comparative study of the role of surface terminal groups on the optical properties, we investigated hydrogen terminated (SiNPs-H) and organic functionalized SiNPs (SiNPs-C12) ensembles with the same mean NP diameter but differing on the surface termination using steady-state and time-resolved photoluminescence at 12 K and 300 K, as well as measurements of the absolute quantum yield at room temperature. The impact of the surface oxidation on the emission features of the SiNPs-C12 was also studied. Both the exciton recombination lifetimes and quantum yields display a pronounced dependence on the surface termination. Exciton lifetimes are found to be significantly lower in SiNPs-H compared to SiNPs-C12. This difference is due to distinct non-radiative recombination probabilities resulting from inter-NP exciton migration, which in SiNPs-C12 is inhibited by the wider energy barriers imposed by the bulky surface groups. This also results in a higher quantum yield observed in SiNPs-C12 compared to SiNPs-H.

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P7 - KERR BLACK HOLES WITH HAIR: SHADOWS, SELF-INTERACTIONS AND OTHER TYPES OF HAIR

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Kerr black holes with scalar hair (KBHsSH) are a new family of Kerr black holes which are solutions of Einstein's gravity coupled to a massive, complex scalar field [1]. KBHsSH have been shown to have distinct phenomenological features when compared to the paradigmatical Kerr black holes, such as their shadow [2].
For KBHsSH, self-interactions can be added and their effects can be found in various phenomenological quantities of interest [3].
Other types of hair, such as massive vector hair, i.e. a Proca field, can also be found around Kerr black holes [4].

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P8 - OCEAN MONITORING WITH SMALL SATELLITES

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One fundamental component of the Earth's ecosystem is the oceans. Traditional methods for ocean monitoring and observation are based on static assets, drifters, or manned ships. However, to understand the changes of ocean features observations over larger spatial and temporal scales are required. To expand the capabilities of traditional methods, robotic platforms have been used, e.g. autonomous underwater vehicles. Although they allow a characterisation of a wider area, in less time and more cost effectively, they are still far from the desired mesoscale (> 50 km2) observation capability. Furthermore, their time of operation is yet limited. Consequently, and for several other reasons, satellite remote sensing is an indispensable tool for Earth Observation, as it is capable to monitor on regional or global scales, and with high spatial and temporal resolution over long periods of time [1].
Starting with mass smaller than 200 kg (e.g. 122kg for the first dedicated weather satellite), spacecraft mass had a natural growth, sustained by the consistent demand on performance. This has direct consequences to their complexity, design, test, launch, operation and cost. With the revolution of very-large-scale integration, the possibility of having sophisticated functions fitted into small volumes, with low mass and power, arose. This revolution lead to the concept of the modern small satellite [2], while their more recent design evolution (lead by the CubeSat standard and other technologies) can prove to be promising for operational remote sensing [3].
One domain on which these platforms have not yet shown their potential, for lack of missions, is in the ocean sciences. Therefore, our work main thesis is that small satellites can be a key element in the (near) future needs of oceanography [4]. The reason for that is not only due to their lower cost and more modest operational requirements. The evolution of autonomous robotic platforms, with smaller form-factor sensors, can be adapted and leveraged for small satellites. Furthermore, as sensors become increasingly affordable, multiple small satellites could be launched to create a constellation of identical spacecraft, all pointing Earthwards with the same set of sensors, to provide near real-time coverage to any part of the planet, especially the remote oceans.
Even though satellites cannot make in situ measurements, their synoptic observations give us a global picture of the oceans. Intelligently combining this with robotic elements, ensuring they are ``at the right place and right time'', to obtain data especially of episodic phenomenon, can considerably boost the study of the oceans, and yield an unprecedented view of our evolving ecosystem on Earth.
Our initial objective was to survey what small satellites capabilities are currently available, and in many cases previously proposed, attempting to give a perspective of the use of such technologies now, and in the near future, for oceanographic measurements.
With that set, our current objective is to add to an autonomous vehicle, developed for oceanographic research, a satellite communication board. In particular, and for now, it will use a CubeSat to send information to a ground station. In the future, these vehicles and satellites can be part of an integrated system for ocean research.

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