Essay Proposals 2019-29

Assigned Proposals

1.Advanced Materials for Radiofrequency Electromagnetic Interference Shielding: Nanomaterials, Patterns and Textiles

Student :*Ana Rita Correia e Sousa (up201204635@fc.up.pt)*

Supervisor: *André Pereira(ampereira@fc.up.pt)*

2. Microfluidics for size-controlled cationic liposome-DNA complexes: going beyond the universal transfection curve,

Student: Celso Joel Oliveira Ferreira (bruno.silva@inl.int)

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3.Topological insulators grown by molecular beam epitaxy (MBE) and related quantum devices

Student: Daniel Portela de Brito (dani_brito96@hotmail.com)

Supervisors: *Eduardo Castro (evcastro@fc.up.pt) ; Sascha Sadewasser (Sascha.Sadewasser@inl.int)*

4. Development of nanoplasmonic thin film biosensors with enhanced sensitivity for detection of mycotoxins

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5. Study of structural liquid water anomaly by upconversion thermometry on Brownian nanoparticles

Student: Fernando Eduardo Maturi (maturi@ua.pt)

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6. Quantum Many-Body Ground States via Digital Quantum Simulation

Student: Bruno Rodrigues Pacheco e Murta (bpmurta@gmail.com)

Supervisor: J oaquín Fernández-Rossier (joaquin.fernandez-rossier@inl.int)

7. *Excitons in van der Waals Heterostructures*

Student: Maurício Fitz de Castro Martins Quintela (mfcmquintela@fc.up.pt)

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8. *Hyperspectral microscopy for molecular thermometry*

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9. *MagMed - Novel magnetic nanostructures as multimodal nanocarriers for cancer therapies*

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10. *Development of multifunctional supramolecular magnetogels for multimodal cancer therapy*

Student: Sérgio Rafael da Silva Veloso (sergioveloso96@gmail.com)

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11. *Fluids of light for analogue computing*

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12. *Trivalent lanthanides ions for luminescent molecular logic*

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13. *Online coupled atmospheric-aerosol regional forecast model for solar energy production*

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Supervisor: Alfredo Moreira Caseiro Rocha (alfredo.rocha@ua.pt); Ana Cristina Caldeira da Silva Gouveia Carvalho(ana.carvalho@smhi.se)

14.*Transparent thermoelectric titanium dioxide-based thin films for thermal energy harvesting*

Student: Joana Margarida Fernandes da Silva Ribeiro (joanaribeiro93@hotmail.com)

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15.*Single Photons On Demand from a 2D Material Heterostructure*

Student: Tiago Alves Queirós (tiagoaqueiros@gmail.com)

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Open Proposals

15.*Calculation of Berry connections from first principles*

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Detailed Descriptions

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Title

Advanced Materials for Radiofrequency Electromagnetic Interference Shielding: Nanomaterials, Patterns and Textiles

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Materials Science, Nanotechnology, Engineering Physics, Electromagnetic Shielding, Electromagnetism,

Summary of Proposal

Upgrading the human lifestyle and technology through the development of modern telecommunications boost concerns regarding the expansion of mobile phones systems, computers and wireless internet. Such technologies need to ensure a certain level of protection against undesirable emission of electromagnetic fields for protecting the human health. Moreover, certain types of people are susceptible to this radiation such as users of pacemakers, stents or implants. Finally, undesirable electromagnetic interference (EMI) can occur from operating devices that can affect the functionality of surrounding devices. Thus, there is a demand for the development of innovative EMI shielding materials. Several applications can be framed within these purposes, such as military applications and wearable textiles for clothing .

The main goals for the present essay proposal are:

- Study of the state-of-the-art concerning the advances on EMI shielding materials; in particular:

- Experimental measurement methods of EMI such Shielding Effectiveness measurement setup assembly and development using squared wave-guides and VNA ;

- The play rule of the nanomaterials on the shielding effectiveness;

- The new trend and innovative EMI shielding materials applying conducting polymers, carbon materials and magnetic nanoparticles: Preparation, characterization and shielding performance measurements ;

- Numerical simulations;

- Application of advanced materials for RF EMI Shielding on textiles ;

This proposal is framed within the scope of the project RFProTex - POCI-01-0247-FEDER-039833. This project involves multidisciplinarity since it brings together Universities, Center for Technological Transfer and Industrial partners.

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Title

Microfluidics for size-controlled cationic liposome-DNA complexes: going beyond the universal transfection curve

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Materials and colloidal science

Summary of Proposal

Cationic Liposome – DNA complexes (also known as lipoplexes) are a type of self-assembled system consisting of cationic liposomes complexed with nucleic acids. The major driving force for lipoplex formation is the high entropic gain due to the release of the inorganic counterions after the nucleic acids (which are negative) and cationic liposomes neutralize each other. Lipoplexes are promising non-viral vehicles for gene therapy, but the poor understanding of their interactions with biological systems leads to low transfection efficiencies (TE). One factor that contributes to such poor understanding is the inability of conventional methods of lipoplex preparation to produce monodisperse and tunable particle sizes. Besides these hurdles, it has been shown that the membrane charge density of lipoplexes is a universal determinant of TE.

It has also been demonstrated that model particles of different sizes interact differently with cells and follow different endocytic pathways. We hypothesize that besides membrane charge density, lipoplex size has also a key role in determining TE. The aim of this project is to develop a microfluidic methodology to produce lipoplexes of controlled and tunable size, and use this technology to understand how membrane charge and particle size control TE. An understanding of these factors will increase our knowledge about the interactions of lipoplexes with biologic systems, and lead to improved formulations for gene delivery.

We have recently demonstrated that microfluidics can be used to produce cubosomes (self-assembled lipid nanoparticles with internal cubic symmetry). The first objective of this proposal is then to (i) implement a similar methodology leading to lipoplexes of controlled size. The second objective of the proposal is to (ii) decouple the size-charge dependence of lipoplexes on the transfection efficiency. As a third objective, we aim to (iii.a) understand how the size and charge influence the interactions of the particles with serum and how these can influence TE; and how (iii.b) PEGylating the particles modulates this behavior. Ultimately, we expect to discover regimes of enhanced TE for therapeutics.

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Title

Topological insulators grown by molecular beam epitaxy (MBE) and related quantum devices

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,….);

Materials

Summary of Proposal

Topological insulators (TIs) are a new family of materials that have received plenty attention due to the prediction of a variety of novel properties. A topological insulator is electrically insulating in the bulk form but possesses highly conductive and spin-polarized massless Dirac surface states that are protected against disorder by time-reversal symmetry, allowing near dissipation-less transport of (spin) charge on the surface [2].

There are many practical challenges limiting the study of the properties of the surface states and their applications. Proper material synthesis is one of them. TIs are usually deposited by the cumbersome exfoliation method, chemical vapor deposition (CVD) or molecular beam epitaxy (MBE); the latter will be the focus of this project.

In TIs, the material structure consists of quantum layers connected by van der Waals forces, which is a weak intermolecular force. The crystal is easy to dissociate between layers under an external force. As graphene, which can be prepared by exfoliating the graphite layer-by-layer, TIs layers can also be obtained by the exfoliation of big single crystals. High-quality TIs can be deposited by CVD [2], wherein a reactant is evaporated at high temperatures and carried by inert gases to the

substrate, usually obtaining a large area of very thin material. Together with CVD, MBE is the standard method for growth of high-quality optoelectronic devices. Differently from CVD, MBE uses pure elements as precursors and the growth occurs in ultra-high vacuum conditions, which has a number of advantages: large-area growth, the ability to control doping, lattice mismatch or defects at the interfaces [1]. In MBE, fine tuning of the growth conditions is possible. However, at the same time, the crystal growth is complex due the extensive parameters to control and the involved physics. The exchange energy with the surface, atomic surface migration, adsorption and nucleation [2] should be considered for proper growth. High quality TIs have been grown successfully by MBE and, through controlled doping, the Quantum Anomalous Hall effect could be observed [3].

The most common TIs are Bi2Se3, Sb2Te3, Bi2Te3, Sb2Se3 and their alloys. Some other materials can show TIs properties upon the application of tension or when incorporated in heterostructures. Very recent studies indicate that the layered semiconductors InSe and GaSe can be transformed into 3D topological insulators by strain engineering [4].

All these materials have a distinguished potential for several devices or applications. At present, the prevalent applications include photodetectors, spin devices, field effect transistors (FETs) and lasers [5]. TI-based photodetectors have high responsivity, fast response time and are wide band (UV to infrared) [6]. TI materials exhibit strong quantum spin Hall effect, and their surface has a spin-related conductive channel. This means that the non-zero spin density flow spontaneously appears when the electrons flow on a TI surface [2], which could be applied for new kinds of spintronic devices. If a ferromagnetic material and the TI are coupled to form a heterojunction, the surface current can be used to control the magnetization, thus developing a new type of spin moment and magneto-resistive devices [2].

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Title

Development of nanoplasmonic thin film biosensors with enhanced sensitivity for detection of mycotoxins

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Materials: Plasmonic thin films; Localized Surface Plasmon Resonance sensors

Summary of Proposal

My proposal aims the development of nanoplasmonic materials, with enhanced sensitivity, for detection of mycotoxins commonly found in wine and grape juice. The detection mechanism will be lbased on the shift of the localized surface plasmon resonance band of Au nanoparticles dispersed in an oxide matrix (e.g. TiO_2, Al_2O_3, etc.), resulting from the interaction between target molecules/ nanoparticles. A combination of environmentally friendly and cost-effective physical vapor deposition (PVD) technique, namely reactive magnetron sputtering, with the glancing angle deposition (GLAD) approach will be used to prepare the films, allowing the preparation of specific architectures (e.g inclined columns, spirals, etc.) that may retain better and easily the mycotoxins (e.g. by tailoring density, porosity) for their recognition and quantification. To tailor the metal nanoparticles morphology (size, shape and distribution), thermal annealing treatments and plasma activation routines will be optimized. After a proper functionalization with chemical linkers (e.g. monolayers with -thiol and -amine groups) and biorecognition elements (e.g. antibodies), the sensor prototypes will be integrated in a high-resolution LSPR spectroscopy system to monitor the LSPR band changes, in the presence of the target molecules.

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Title

Study of structural liquid water anomaly by upconversion thermometry on Brownian nanoparticles

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Optics

Summary of Proposal

Despite its simple molecular structure, liquid water is one of the most fascinating and complex substances. There are many questions regarding liquid-liquid water transitions, which are subtle to observe experimentally. In this way, the main goal of this proposal is the study of the anomalous behavior of liquid water through temperature-dependent photoluminescence by upconversion thermometry using lanthanide-doped nanoparticles. The use of trivalent lanthanide ions (e.g. ytterbium and erbium) allows the measurement of temperature without external calibration, which is suitable for studying temperature-induced changes in the aqueous medium. The effect of solvent and temperature increase on the instantaneous Brownian velocity of nanoparticles suspended in water pave the way for gathering information about the hydrogen-bonding network of the liquid water around the nanoparticles.

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Title

Quantum Many-Body Ground States via Digital Quantum Simulation

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Theoretical Condensed Matter Physics

Summary of Proposal

The quantum many-body problem cannot be solved generally in conventional hardware due to the exponential scaling of memory resources with the number of degrees of freedom [1]. This hampers our understanding of several areas in condensed matter physics, particularly those involving strong interactions. Fault-tolerant quantum computers are expected to provide a way around this exponential wall problem [2]. In fact, quantum simulation is one of the leading candidate applications where the long-awaited quantum supremacy [3] – the ability to solve on a quantum computer a problem deemed unsolvable by classical hardware – may be achieved.

Given a many-body Hamiltonian, its ground state can be obtained via quantum phase estimation [4] provided that a state with non-negligible overlap with the ground state can be prepared (e.g. via adiabatic state preparation [5]). However, the computational resources required to implement this procedure are far beyond the capabilities of near-term quantum computers [6,7]. Indeed, state-of-the-art quantum hardware is currently limited by the small number of available qubits and the short timescales over which quantum operations can be performed coherently [8].

Within this context, hybrid quantum-classical methods have taken the spotlight, thanks to the decomposition of an otherwise deep quantum circuit into many independent shallow ones and the delegation of the optimization procedure to classical hardware. The leading algorithm, particularly to tackle the electronic structure problem, is the Variational Quantum Eigensolver (VQE) [9]. It comprises two subroutines: 1) a quantum computer prepares a parameterized wave function ansatz and measures the expectation value of the Hamiltonian given the parameters; 2) a classical computer runs an optimization algorithm that sets the parameters.

The success of VQE is largely dependent upon the choice of ansatz. Most ansätze proposed in the early days of this field were based on the Unitary Coupled Cluster (UCC) [10] method, but could only be successfully applied to simple molecular chemistry problems [9,11] because larger systems admit many possible excitations, yielding deep quantum circuits. As an alternative, hardware-efficient ansätze were proposed [12], but face two issues [13]: first, the trial states produced by these ansätze cluster on barren plateaus in the Hilbert space, with energy close to the average of a totally mixed state; second, the gradient is zero along most directions of this space, making the parameter optimization difficult. The search for ansätze suited for larger systems with strong interactions has been an active field recently, including an adaptation of UCC to quasiparticle operators [14] and the so-called Hamiltonian variational ansatz [15].

The first part of the project hereby proposed is to explore the full potential of near-term quantum processors to simulate strongly correlated systems in low dimensions. In particular, the candidate will develop quantum algorithms to implement ansätze used in classical variational schemes – including (but not restricted to) the Gutzwiller wave function [16], matrix product states [17] and projected entangled pair states [18] – on near-term quantum computers, taking hardware limitations into account.

In light of the ongoing rising trend in qubit coherence times [19], it is foreseeable that, within 5 to 10 years, quantum hardware resources will be sufficiently abundant to go beyond hybrid variational algorithms. At that point, adiabatic state preparation [5] will be feasible, allowing to overcome the inherent limitations of VQE [9] or quantum phase estimation with an initial mean-field state [4], notably the infamous orthogonality catastrophe [20]. Nevertheless, it is unlikely that full fault tolerance will be achieved due to the large overhead imposed by quantum error correction schemes [21]. Optimizing the quantum circuit depths will therefore still be a crucial practical challenge.

In the second part of this project the candidate will develop strategies to optimize adiabatic state preparation in quantum hardware. Specifically, the resources required to implement each time step of the propagator, on the one hand, and satisfy the adiabatic condition [5], on the other, will be minimized. The implementation of adiabatic state preparation in quantum hardware to prepare the ground state of canonical interacting spin and fermionic systems will also be considered.

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Title

Excitons in van der Waals Heterostructures

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,….*);

condensed matter physics, optoelectronics

Summary of Proposal

Alongside graphene (first mechanically exfoliated in 2004 by Novoselov and Geim), a wide range of bi-dimensional materials are currently studied and have a plethora of different physical properties and applications. An important subclass of these materials is the family of transition-metal dichalcogenides with chemical formula MX2, where M is a transition metal and X a chalcogen atom. These materials, specifically those with group-VI transition metals, are semiconductors which exhibit strong light-matter coupling, as well as having direct band gaps in the infrared and visible spectral regimes (demonstrated independently by Heinz and Wand in 2010). These properties make them good candidates for various applications in optics and optoelectronics.

The optical response of these semiconductors is mainly dominated by the excitation of electrons from the valence band to the conduction band. Such a phenomena can be described by a pair of interacting (effective) particles, one being a conduction electron and the other being a hole left in the valence band, with opposite charge to the electron. Considering frequencies above the band gap, a transition from the valence to the conduction band is possible, which means that the absorption becomes finite. For certain materials, absorption peaks can be measure below the band gap, which can be explained by the presence of excitonic states.

As the electron and hole are particles of opposite charges, the most natural formulation of their interaction will be a Coulomb potential. This will lead to the possibility of the formation of bound states between these particles, analogous to those formed between an electron and a proton in the hydrogen atom. This analogy makes it so that the study of the hydrogen atom in different scenarios (confined in a region (Aquino-2005, Chaos-Cador-2005), or inserting a minimum distance into the Coulomb potential, for example) can be elucidative in both the the obtained results and the applicable methods. Unfortunately, the small mass of the particles in question and large screening effects means that the excitonic binding energy in bulk materials is of the meV scale, while the room-temperature thermal fluctuations are about 25 meV. These fluctuations mask excitonic effects unless the material is sufficiently cooled down.

In transition-metal dichalcogenides (TMDs), where the screening effect is reduced, the exciton binding energies reach values the order of 100 meV. Therefore, these class of excitons are more easily accessible to experimental study, as they are observable at room temperature. As an example, WSe2 in a fused quartz substrate presents two excitonic peaks in the linear absorption at 1.65 and 2.08 eV. These peaks, however, were not consistent with the Coulomb interaction, which shows the necessity of including screening effects in the electron-hole effects.

The simplest way of including a screening-like effect is via the soft-Coulomb potential, which introduces a material-dependent minimum separation-like parameter between the electron and the hole. Another of these potentials is the Rytova-Keldysh potential, which includes a material dependent parameter and reduces to the Coulomb potential the regime where this parameter is zero. Mathematically, this potential is significantly more complex than the Coulomb potential, which in turn further complicates the analytical work in determining the absorption spectrum.

Another relevant aspect are spatially separated excitons, where each element of the electron-hole pair is situated in a different layer. These excitons as specially relevant in van der Waals heterostructures, where multiple layers of different TMDs are stacked. With the previously-mentioned soft-Coulomb potential, this bias distance is easily introduced as a minimum separation parameter, which depends on the specific heterostructure. The obtained theoretical results (from either variational or numerical methods) can be compared with experimental results, where the minimum separation is usually of the order of the effective Bohr radius for an electron-hole pair in the material in question.

Besides van der Waals heterostructures, where the screening effects reflect the nature of the different materials in each layer, these same screening effects are fundamental when one wishes to study TMD monolayers surrounded by a dielectric medium with a dielectric constant different from that of the TMD. In these systems, as mentioned before, the physics of the electron-hole is better modeled by replacing the Coulomb potential with the Rytova-Keldysh potential with parameters related to the relative dielectric constants of the media surrounding the monolayer, as well as the 2D polarizability of the TMD.

In this PhD project, we will be using both numerical and analytical methods. For excitons in bulk structures, much analytical progress can be made, while for spatially-confined excitons in van der Waals quantum dots (discussed, for example, by Andrea-1990 and Rana-2014) most of the work will be numeric. The idea is to expand the solution of the Wannier equation in a convenient basis and diagonalize the corresponding eigenvalue problem. The eigenvalues will give the binding energies of the excitons and the eigenvectors the corresponding wave functions. Both of them will be used for computing the absorption and the polarizability. The approach to the calculation of the Stark effect and ionization rate (discussed, for example, by Scharf-2016 and Massicotte-2018) will be done both analytically and numerically (only discussed in van der Waals heterostructures by one published paper so far, by Kamban in 2020). In the analytical approach we will use semiclassical methods, which have recently proven quite powerful in this context, whereas in the numerical methods a number of approaches are available for separable potentials. For non-separable potentials, other methods have to be used, such the complex coordinate scaling approach. Thus the PhD project will develop a suite of numerical methods that can be used in other system to be discovered in the future.

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Title

Hyperspectral microscopy for molecular thermometry

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Optics

Summary of Proposal

Hyperspectral microscopy is a technique that can be used to simultaneously obtain spectral and spatial information by combining spectroscopy with optical microscopy. [1,2] Such a combination allows us to capture images with a spectral resolution of up to 2.73 nm in a spectral range of 400 – 1000 nm with a spatial resolution in the submicron scale. The relevance of hyperspectral imaging for mapping at the submicron scale [3] has been described in a few reports focused on biomedical applications, such as cellular uptake monitoring [4-8] of bioimaging agents and identification of pathogens and cancerous cells. [9-13] In these examples, the spectral profile results from light reflectance measurements. The combination of hyperspectral microscopy with photoluminescence measurements is even less explored and, as far as we know, only two examples were published. One refers to down-shifting Si-based NPs whose emission in the red spectral range combined with hyperspectral analysis was used to discuss film homogeneity at the submicron scale [14] and the other example explores hyperspectral microscopy within MG-63 cells in which the emission arising from UCNPs enabled the monitoring of cellular uptake in lanthanide-based NPs. [15]

The main goal of this thesis is to develop a 3D temperature mapping at submicron scale using luminescent nanothermometry and lanthanide-based upconverting nanoparticles (UCNPs) as emission probes. The emission spectra of UCNPs acquired using a Cytoviva hyperspectral microscopy system available at Phantom-g, Department of Physics of University of Aveiro, with spectral resolution up to 2.73 nm in a spectral range of 400 – 1000 nm with a spatial resolution in the submicron scale. Each image will be acquired in planes, with each pixel of hyperspectral image measuring $(12.9/M)^2$ μm^2, where M is the objective magnification (up to 100x). In order to obtain the 3D temperature mapping, a piezo-driven platform in the Z-axis will allow the image acquisition in different planes. Having this set of images, a protocol is expected to be developed to obtain the 3D temperature mapping.

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Title

MagMed - Novel magnetic nanostructures as multimodal nanocarriers for cancer therapies

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Medical Physics

Summary of Proposal

Almost one and a third million people died from cancer in Europe in 2015, which equated to more than one quarter (25.4 %) of the total number of deaths. Current oncologic therapies are commonly associated with undesirable side effects, due to their cytotoxicity and poor tumor targeting. A major advance in therapy could be achieved if drug carriers presented an efficient dual triggering: treatment and transport/release of the drug at the target tumor site. In this context, this project aims to develop a novel multimodal generation of targeted nanocarriers, loaded with anticancer drugs and combined with a magneto-mechanical action through a magnetic core. Beyond the use of classic magnetic spherical nanoparticles, novel and promising nanodiscs with unique spin configurations, synthetized by template-assisted nanofabrication and lithography, will be optimized. Lipid nanoparticles will be used as a shell due to their biocompability, surface properties that can be modulated for targeting, high drug payload and reduced absorption via lymphatic system, which improves drug bioavailability.

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Title

Development of multifunctional supramolecular magnetogels for multimodal cancer therapy

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Nanomaterials

Summary of Proposal

In this project, magnetic nanoparticles based on transition metal ferrites ($X_nY_{1-n}Fe2O4$ (X= Ca, Mg; Y= Co, Mn; n = 0.25-0.75)) will be developed, characterized and combined with a silica, gold or lipid shell. This will allow improved biocompatibility, enhanced hyperthermia efficiency and/or photothermia capability. Supramolecular peptide-based hydrogels containing cyclic-RGD and IKVAV will be synthesized and combined with magnetic nanoparticles into magnetogels, which will be structurally and mechanically characterized. The developed magnetogels will be evaluated as nanocarriers for the controlled release of anticancer drugs by assessing the interaction with biomembrane models and drug release kinetics. Magnetic hyperthermia and photothermia potentialities on local heating and drug release will be studied through application of external alternating magnetic field and/or plasmon irradiation of gold containing nanoparticles. Hereby, this project aims at developing biocompatible soft magnetic nanomaterials capable of improving cancer therapy efficiency through the synergy between chemotherapy and hyperthermia/photothermia.

Concerning the requirement for better patient's quality of life, target specificity, therapeutic effectiveness and lower cost as a major problem to solve, not only to reduce the adverse effects on healthy cells but also to extend better and affordable treatments to low-income countries, this project aims at guaranteeing quality health access and promote the well-being for all ages (goal 3 of the 2030 Sustainable Development Agenda) by accomplishing the following objectives:

-Preparation and characterization of spherical and anisotropic magnetic nanoparticles based on mixed metal ferrites with and without coating with silica, gold or lipids;

-Synthesis and characterization of new supramolecular peptide-based hydrogels;

-Development and characterization of hydrogels bearing the developed nanoparticles;

-Development and characterization of mixed hydrogels and magnetogels with the active functionalities to favor cell growth and active targeting;

-Conceptualization and development of magnetonanolipogels, consisting of hydrogels containing solid magnetoliposomes and magnetoliposomes containing stimuli-responsive hydrogelators;

-Evaluation of the nanosystems as potential nanocarriers for commercial chemotherapeutic drugs.

-Evaluation of the nanosystems potentiality as multimodal therapeutic agents by magnetic hyperthermia or photothermia and drug delivery;

-Publication of results and reviews in ISI journals, oral presentations, and posters in international and national conferences.

(*continue if necessary*)

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Title

Fluids of light for analogue computing

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Nonlinear quantum optics, many-body systems, analogue computing, fluids of light

Summary of Proposal

The essay aims to provide an overview of the state-of-the-art relevant of quantum optical systems experimentally accessible that can be used as platforms for analogue quantum computing [13] using light to emulate phenomena and systems that are hard or even impossible to investigate in the laboratory under controlled conditions. We focus our attention on tunable coherent quantum-optical many-body systems (e.g. nematic liquid crystals[1], thermo-optical media[5,14], photonic-fluids[15], atomic-media[2,16], ultracold, Rydberg and Bose gases[17], graphene[8]), which are excellent support for optical analogues capable of exploring the fundamental properties of other quantum systems, ranging from superfluidity of light[1,2,3.4], Boson-stars[6,14,18], dark-matter[5], gravitating Bose-Einstein condensates[18], quantum gravity[6], gravitational effects[19] and Hawking radiation [7]. This review provides an opportunity to discuss the fundamental models describing these systems, the type of phenomena that they can support (e.g. thermalization[11], interference[12], transient and relaxation processes at the microscopic scale in QOMBS[11,16], macroscopic quantum effects[1,9,10]), and how they can be explored within the context of the thesis program, especially for quantum analogue computing.

As a guideline for the preparation of the essay, we provide a list of topics that can be addressed:

1.Fluids of light and exotic states of light in strong light-matter interaction regimes: theoretical framework

Part I. Analogue systems

2.Quantum fluids of light

3.Quantum simulation and analogue computing

4.Applications of analogue computing: superfluidity, analogue gravity, dark-matter, etc.

Part II Optical media

5. Nonlinear local media

6. Nonlinear nonlocal media

7. Other materials that may support exotic states of matter (e.g. liquid crystals, nonlinear photonic crystals, polaritons, atomic gases)

Part III Thesis proposal

(*continue if necessary*)

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Title

Trivalent lanthanides ions for luminescent molecular logic

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Optics

Summary of Proposal

The evolution of the internet of things, the digitalization to networking is increasing the demand for computing power as a technological challenge. Nowadays, modern Si-based chip architectures are moving closer to the limits of what is physically feasible by the top-down lithographic approach, stressing that a step forward towards a bottom-up approach is desirable to face the demand for higher miniaturization [1]. Therefore, the current ongoing belongs to nanostructured materials where a proper structure is obtained by means of bottom-up nanotechnology.
These new challenges require a new generation of computing systems distinct from those exploited in nowadays state of art computers [2]. In early 90's, the pioneering works of Prasanna da Silva et al. inspired a first general and practical approach to information processing and computing based on molecules able to perform logical operations [3]. Since then, the research

field grows studying systems essentially based on organic molecules and exploiting chemical inputs [4].

Despite it is nowadays recognized that Ln3+ ions can improve the state-of-the-art of molecular logical devices, only a few works have been reported so far. In mostly of the them, the Ln3+ ions respond to chemical inputs and the molecular logical devices operate exclusively in wet conditions. Recognizing the huge potential of molecular logical devices based on Ln3+ ions emission, and the possibility of multiplexing the narrow emitting lines and for parallel processing, the goal of this thesis is to develop molecular logic devices exploiting the Ln3+ ions as active computing centres and using preferentially physical inputs [5][6]. This work will explore several possibilities to modulate the excitation sources (pulse width, frequency, start delay, power density) as physical stimuli that will permit the systems to perform different binary arithmetic operations and even more complex logical operations including the possibility perform of storage the information.

(*continue if necessary*)

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Title

Online coupled atmospheric-aerosol regional forecast model for solar energy production

Area

Meteorology and Climate

Summary of Proposal

Solar radiation has been explored for energy purposes as a renewable energy source. The installation and running of solar energy systems require a good solar radiation climatology and radiation forecast. Such information has been obtained to a great extent using atmospheric numerical models. However, the aerosol interaction with radiation and clouds is frequently omitted in these models. The radiative forcing of aerosols can be considerable under particular conditions. It is now established that atmospheric aerosols must be included in models to improve NWP and climate simulations. Despite the existence of studies on the feedback mechanisms related with aerosols, there are still scientific questions to answer regarding their influence on the radiation budget, atmospheric dynamics and thermodynamics. The work proposed here intends to include aerosols in NWP and climate models by implementing an online coupled atmospheric-chemistry model for the Iberian Peninsula to improve radiation simulation at the surface for energy production.

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Title

Transparent thermoelectric titanium dioxide-based thin films for thermal energy harvesting

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Materials

Summary of Proposal

This project envisages the study, development, characterization and application of TiO2–based thin films which are transparent in the visible region and show thermoelectric properties. These films have the potential to efficiently harvest thermal energy from the environment and convert it to electricity. In this project, TiO2 (titanium dioxide) films ($\sim$100 nm thick) doped with metal cations such as Nb or Bi will be deposited on glass and Si substrates by reactive magnetron sputtering in high vacuum. The films will be thoroughly characterized so that several process parameters can be adjusted, such as reactive and working gas partial pressures, deposition temperature, target current density, substrate biasing and post-annealing conditions. These parameters directly affect the morphology and crystalline structure of the thin films. Hence, modifying their optical, electric, thermal and thermoelectric properties enables their suitability for application as thermal energy harvesting devices in photovoltaic systems, touch displays, amongst other devices, to render these more sustainable.

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Title

TSingle Photons On Demand from a 2D Material Heterostructure

Area

(*Materials, Optics, Condensed Theory, High Energy Theory,....*);

Quantum materials for quantum science and technology

Summary of Proposal

Single-photon emitters are essential components for the realization of quantum devices, e.g.,quantum key distribution, quantum repeaters, and quantum information processing. Single-photon generation was achieved in single molecules, quantum dots, color centers in diamond, and recentlyin 2D materials, e.g., in hexagonal Boron Nitride (hBN).

We propose to fabricate a device based on a 2D materials heterostructure consisting of an hBN layercontaining point defects acting as single emitters on top of graphene patches, which can beindividually addressed and gated, thus controlling the emission state of the defect. The single-photon emitters are switched to open and closed states, through the modulation of graphene's Fermilevel that will Pauli block (open) or allow (close) the electronic transitions in graphene responsiblefor the near-field quenching of the emitters. A first application of the developed proof-of-principle device will be explored in the area of cellular quantum bio-imaging.

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Open Proposals

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Calculation of Berry connections from first principles

Area

(*Materials*, *Optics*, *Condensed Theory*, *High Energy Theory*,....);

Condensed Matter Theory

Summary of Proposal

Berry geometries are a hot topic in condensed matter physics, and they can be calculated from the Berry connections.

A set of programs in pyhton and fortran have been developed recently that calculates the Berry connections from first principles and optical properties up to second order using the Berry connections.

The proposal is to further develop the software to incorporate more types of materials (up to now, only some 2D materials with no spin are available) and more properties to be calculated.

(*continue if necessary*)

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(to *allow students first look at topic*)

Vanderbilt, "Berry Phases in Electronic Structure Theory"