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Title of the project: Optoelectronic properties of ZnO-based light-emitting devices

Name of the Group: *Group of Optoelectronics and Photonics (Faculty of Physics)*

Short description of the project: Light emitting devices will be design, fabricated and characterized during the execution of the Master thesis. Oxide semiconductors compatible with silicon technology will be employed as active material, such as SiO2 or ZnO alloyed with nitrogen. The inclusion of rare ions will be also considered as optically active centers. Electroluminescence emission, quantum efficiency and modulation properties of the devices will be studied and modeled. PhD studies are possible after the master thesis.

Contact persons:
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Dr. Sergi Hernández Márquez, shernandez@ub.edu

Title of the project: Electrical study of the resistive switching properties of metal oxide (ZnO-based) compounds

Name of the Group: *Group of Optoelectronics and Photonics (Faculty of Physics)*

Short description of the project: Materials based on silicon and transition metal oxides will be employed for fabricating resistive switching devices (memristors), using a simple metal-oxide-semiconductor (MOS) configuration. The electrical I(V) curves of the devices will be studied by applying a voltage on the top electrode while grounding the bottom contact, sweeping it from negative to positive voltages. The charge transport mechanisms will also be analyzed for the different resistance states (pristine, high resistance and low resistance states), with the aim of obtaining information regarding the mechanism that drives the resistive switching process. PhD studies are possible after the master thesis.
Contact persons:
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Topic: Preparation and study of multifunctional molecules for spintronics

Name of the Group: *Grup de Magnetisme i Molècules Funcionals (GMMF) (Faculty of Chemistry)* http://www.gmmf-ub.com/

Contact person: Dr. Guillem Aromí (aromi@ub.edu)

Title of the project: Study of 3D neuronal cultures alteration by Amyloid-magnetite complex for a better understanding of Alzheimer disease

Name of the Group: *Unitat Bioelectrònica del Laboratori de Nanobioengenieria (www.ibecbarcelona.eu)*

Description of the project: Abnormal accumulation of iron in the brain has been observed in Alzheimer's disease (AD), Parkinson's disease, Huntington's disease, and multiple sclerosis [1]. In AD, the binding of iron to monomers, oligomers, or fibrils of amyloid β peptide (Aβ), the main component of the characteristic extracellular plaques formed in the brain, has been proposed as a mechanism that stabilizes $Fe2^{+}$ and $Fe3^{+}$ ions and favors the formation of free radicals that could provoke the death of neurons by apoptosis [2].
Our research group has focused some effort in reveling the association of magnetite nanoparticles and Aβ in vitro [3], the properties and size of the magnetite nanoparticles formed in the presence
of Aβ [4] and the higher toxicity of magnetite-Aβ complex tested in 2D neuronal cultures [5]. But we want to go a step beyond and study neuronal toxicity of this complex in 3D cultures. 3D cultures bring more adequate representations of cell environment and permits cells to grow and interact in all directions, similar to how they would in vivo. This improved cell contacts with their environment let to achieve more realistic cell-cell and cell-matrix interactions, complex transport dynamics, cell migration, differentiation and survival.

Task. 1. Thioflavin test to monitor the Aβ fibrils structure under different concentrations of $Fe2^{+}$ and $Fe3^{+}$ ions
Task. 2. 3D-neuronal cultures fabrication in collaboration with a group expert in this field.
Task. 3. Toxicity test of neuronal cells under different concentration/Aβ fibrillation
Task 4. Different type of immune staining to determine the type of cells affected by the magnetite- Aβ complex.

Requirements;
It is recommended that the applicant has a background in biotechnology or biology, good English skills, strong initiative and curiosity, skillful and good team worker

[1] Ke Y, Qian Z. Iron misregulation in the brain: a primary cause of neurodegenerative disorders. Lancet Neurol 2003;2:246-53.
[2] Smith MA, Harris PLR, Sayre LM, Perry G. Iron accumulation in Alzheimer disease is a source of redox-generated free radicals. Proc Natl Acad Sci U S A 1997;94:9866-8.
[3] Mir M, Tahirbegi IB, Valle-Delgado JJ, Fernàndez-Busquets X, Samitier J. In vitro study of magnetite-amyloid β complex formation, Nanomedicine, 2012, 8 (6). 974-980.
[4] Teller S, Tahirbegi BI, Mir M, Samitie J, Soriano J. Magnetite-Amyloid-β deteriorates activity and functional organization in an in vitro model for Alzheimer's disease, Scientific Reports, 26 (5), 2015, 17261-16
[5] Tahirbegi IB, Pardo WA, Alvira M, Mir M, Samitier J. Amyloid Aβ42, a promoter for magnetite nanoparticles formation in Alzheimer's disease, Nanotechnology, 2016, 27, 465102-465109

Contact person: Dr. Mònica Mir, +34 934 037 178, mmir@ibecbarcelona.eu

Title of the project: Early detection of circulating tumour biomarkers in situ with implantable vascular sensor

Name of the Group: *Unitat Bioelectrònica del Laboratori de Nanobioengenieria (www.ibecbarcelona.eu)*

Description of the project: Cancer is the second cause of death in the world. However, the methods for the advanced prognosis of this disease are nonexistent, being the pathological examination the current standard. Once the tumor is detected, invasive tissue extraction is required by solid biopsy to determine the type of cancer. The discovery of biomarkers in the blood of cancer has revolutionized oncological diagnosis, offering an early method of painless and non-invasive cancer detection [1].
The objective of this project is to develop a diagnostic platform through liquid blood biopsy, for the analysis of biomarkers of cancer in circulation, allowing an early prognosis of this disease at low cost, easy to use, portable, non-invasive and painless. This platform, in addition to performing early prognosis, allows monitoring the evolution of the disease, offering the possibility of providing personalized therapy to the patient. This diagnostic platform will be miniaturized to be implanted through a needle into the bloodstream. This system allows on-site detection in real time, accessing the entire concentration of biomarkers in the patient. Nanostructured polymeric structures will be studied to further increase sensitivity in detection. To avoid the use of animals in the validation of this technology and to have an in vitro system of easy use and low cost, a microfluidic system will be developed to mimic the implantation and the conditions in which the sensor will be found in the branchial artery.

Task. 1. Positively charged polymers for DNA entrapment
Task. 2. Tuning of Polymers porosity for entrapment enhancement
Task. 3. Fluorescent test of the entrapped DNA under batch conditions
Task 4. Microfluidics fabrication and test of the entrapment under in vivo conditions
Task 5. Potentiometric test of the entrapped DNA
Task 6. PCR test for limit of detection improvement of the DNA entrapped

Requirements;
It is recommended that the applicant has good English skills, strong initiative and curiosity, skillful and good team worker

[1] José Marrugo-Ramírez, Mònica Mir, Josep Samitier, Blood-based cancer biomarkers in liquid biopsy: A promising non-invasive alternative to tissue biopsy, International Journal of Molecular Science, 2018, 19 (10), 2877.

Contact person: Dr. Mònica Mir, +34 934 037 178, mmir@ibecbarcelona.eu

Title of the project: Therapeutic Applications of Stimulus Triggered Delivery Systems

Name of the Group: *Resposta Cel·lular als Xenobiòtics (CEREX) (Faculty of Pharmacy and Food Sciences)*

Description of the project: The procedure by which a drug is administered has a significant effect on its therapeutic efficacy. Some drugs present an optimum concentration range within maximum benefit, and concentrations above or below this range may be toxic or produce no therapeutic benefit.
In order to minimize the degradation of the drug and its loss of efficiency, our research group develops nanoparticle systems for the encapsulation and controlled release of molecules of therapeutic interest. Among other strategies, these systems are designed based on their

response to endogenous stimuli to facilitate the controlled release of the drug. Encapsulated molecules include nucleic acids, proteins and antitumor drugs, among others.
During the development of these systems it is essential to increase their stability in the biological environment, transport, directionalization and interaction with biological barriers. The evaluation of the biocompatibility and cytotoxicity of the nanoparticles systems is key in the modulation of pathophysiological processes.

Contact person: Dr. M. Carmen Morán Badenas (mcmoranb@ub.edu)

Title of the project: Iron oxide nanoparticles for targeted cancer therapy

Name of the Groups: *Grup de Magnetisme i Molècules Funcionals (Faculty of Pharmacy and Food Sciences) http://www.gmmf-ub.com & Grup de Terapia anticancerosa, Immunomodulació i Nutrigenòmica (Faculty of Pharmacy and Food Sciences) http://www.ub.edu/terapiamol/cancer/*

Description of the project:
Iron oxide nanoparticles (NPs) can be readily prepared by well-known methods as monodisperse, crystalline nanoparticles. By controlling the conditions, the major phase in these nanoparticles is the magnetic oxide magnetite, Fe_3O_4. The properties of iron oxide NPs make them excellent candidates for medical applications: Fe is an essential element and iron oxides can be readily metabolized or assimilated by the organism, thus iron oxide NPs lack the toxicity often related to heavy metals. The fact that they are magnetic can be exploited for targeting specific sites in the organism using a magnetic field that is not harmful.

Cancer therapy with PPRH hairpins. PolyPurine Reverse Hoogsteen hairpins are a new kind of gene silencing molecules developed in our laboratory. They consist of two strands of DNA linked by 5 thymidines. Each strand of that DNA is formed by polypurines and bind to each other by Hoogsteen bonds. These hairpins bind to polypyrimidine tracks present in the genomic DNA inhibiting transcription and splicing thus causing a decrease in gene expression. Therefore, this genomic tool can be used to decrease the expression of genes that are overexpressed in certain diseases, such as cancer.

In this project you will work in a multidisciplinary environment. The main goal is a preliminary study of the functionalization of iron oxide NPs with a PPRH hairpin in order to obtain hybrid nanoobjects suitable for delivering the hairpin to the target. The final aim is to be able to deliver therapeutic molecules such as PPRHs using Iron oxide NPs for efficient targeted cancer therapy.

Contact persons: Dr. E. Carolina Sañudo esanudo@ub.edu; Dr. Carles Ciudad cciudad@ub.edu

Title of the project: Exploring the deconstruction and modification of cellulosic materials by enzymatic assisted interactions.

Name of the Group: *Microbial Enzymes for Industrial and Environmental Applications* (http://www.ub.edu/enzimsmicrobians/) *(Faculty of Biology)*

Description of the project: Nowadays, we are working on the biotransformation of natural polymers like cellulose from plants, including the development of enzymes that catalyse their modification, hydrolysis, and/or synthesis. In addition, we are exploring the potential of bacterial cellulose, as an innovative source for new applications, including its utilization as a platform for anchoring proteins, antimicrobial agents and other functionalization. The project involve the study of cellulases and Lytic polysaccharide monooxygenases in cellulosic materials, to oxidize and functionalize sustainable materials.

Contact person: Dr. Susana V. Valenzuela, (susanavalenzuela@ub.edu)

Title of the project: Water-soluble gold nanoparticles for the efficient delivery of DNA in cancer gene therapy

Name of the Group: *Supramolecular Systems in Nanobiomedicine (Faculty of Pharmacy and Food Sciences)*

Description of the project: In this project, small, water-soluble GNP will be synthesized and functionalized with appropriate cationic chemical entities that could work as binders of DNA Polypurine Reverse Hoogsteen hairpins (PPRHs), a novel, effective, and stable approach for gene therapy. The functionalized GNP and their complexes with will be characterized using different techniques (UV-VIS spectroscopy, TEM, SEM, DLS, etc.) and cytotoxicity studies of the suitable GNP and their complexes with PPRH will be performed in various kinds of cancer cells for evaluating their therapeutic efficacy.

Contact person: Dr. David Limón Magaña (davidlimon@ub.edu)

Title of the project: Design and characterization in optical cavities and optomechanical structures

Name of the Group: *Group of Optoelectronics and Photonics (Faculty of Physics)*

Short description of the project: Rare earth-doped glass spherical micro- and nanosphere resonators are structures that show special resonant modes called whispering gallery modes (WGM), which can be used in optical pumping to achieve lasing. On the other hand, optomechanical coupling is taking advantage of the momentum carried by photons to force mechanical motion to an object. In this proposal, optical cavities integrated with silicon technology will be designed, fabricated and tested, in order to understand and exploit the interaction between light in optical cavities and mechanical structures, at the micro- and at the nano-scales.

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Title of the project: Simulation of photonic crystals based on silicon nanopillars

Name of the Group: *MIND - Nanosystems, Dept. of Electronic and Biomedical Engineering (Faculty of Physics)*

Short description of the project: The periodic layouts of dielectric nanostructures can lead to the material behaving as a photonic crystal. Among the possible layout distributions, in this work we propose studying periodic hexagonal structures of silicon nanopillars, simulating the structure by introducing defects and/or other photonic elements (such as resonator rings, wave guides, etc.) and finally , the deformations of the pillars upon the application of external forces.

Contact persons: Elena Lopez-Aymerich, Dr. Albert Romano-Rodriguez (albert.romano@ub.edu)

Title of the project: Development and test of gas nanosensors of gas based on semiconducting oxides

Name of the Group: *MIND-Nanosystems, Dept. of Electronic and Biomedical Engineering (Faculty of Physics)*

Short description of the project: The actual society generates high gas emissions that can be harmful both to health and environment. This fact fosters the development of gas sensors that allow monitoring these emissions with the aim of their control. In this work, we propose to manufacture and study the response of gas nanosensors based on nanostructured metal oxides. The student will participate in the manufacturing and characterization of both materials and devices, as well as the study of the response to some gases of interest in health and environment, such as CO and NO2.

Contact persons: Guillem Domènech-Gil, Dr. Albert Romano-Rodriguez (albert.romano@ub.edu)

Title of the project: Surface-Enhanced Raman Scattering (SERS) biosensors based on self-assembled monolayers of gold nanoparticles

Name of the Group: Self-Organized Complexity and Self-Assembled Materials. SOC&SAM: http://www.ub.edu/socsam/cms/ *(Faculty of Chemistry)*

Short description of the project: Nanoparticle self-assembly is a robust and versatile strategy for the development of functional nanostructured materials, offering low-cost and scalable methods that can be fine-tuned for many different specific applications. SERS is an extremely sensitive technique for the detection of analytes, although current devices lack suitable homogeneity and reproducibility. In this project, custom-synthesized gold nanoparticles of different sizes and shapes with be self-assembled as monolayers by means of the Langmuir-Blodgett technique with tunable lateral density of SERS hot-spots. The devices will be tested in microfluidic environments for the in-situ detection of water pollutants.

Contact person:

Dr. Jordi Ignés Mullol (jignes@ub.edu)

Title of the project: Synthesis and nanostructuration of single-molecule magnets

Name of the Group: *Grup de Magnetisme i Molècules Funcionals. GMMF*: http://www.gmmf-ub.com (*Faculty of Chemistry*).

Short description of the project: Lanthanide single molecule magnets (SMMs) are now on the fast track for implementation of molecular spintronic devices, in particular after discovery of an organometallic SMM that shows hysteresis above liquid nitrogen temperature: an SMM can be operational at a temperature that is technologically easy to achieve, this is an very important breakthrough in the field since up until now all SMMs were only operational at liquid Helium temperatures (Layfield et al. Science, 2018). For molecular spintronics, SMMs must be manipulated and deposited on surfaces.
In this project you will work in a multidisciplinary environment. The main goal is the synthesis of new lanthanide SMMs and their deposition on surfaces.

Contact person: E. Carolina Sañudo (esanudo@ub.edu).

Title of the project: The enigmatic PGE-bearing nanofibers from the Loma Larga Ni-Laterite Deposit (Dominican Republic) - Do they have a geomicrobiological origin?

Name of the Group: *Mineral Resources Research Group (Faculty of Earth Sciences)*

Short description of the project: Enigmatic fibrous platinum-group minerals (PGM) were found within a chromitite body included in limonite from Ni-laterites in the Dominican Republic. These fibrous PGM have a Ru-Os-Ir-Fe dominated composition and are characterized by fibrous textures with grain-forming fibers which are significantly longer (1–5 µm) than wide (~100 nm). These fibrous PGM show numerous complex textures on its surface which are suggestive for neoformation processes: (i) features suggesting growth of platinum-group elements (PGE)-bearing nanofibers; (ii) occurrence of PGM nanoparticles within film material (biofilm?) associated with PGE-bearing nanofibers; (iii) a Si-rich and crater-like texture hosting PGM nanoparticles and an Ir-rich accumulation of irregular shape; (iv) complex PGM nanoparticles with ragged morphologies, resembling sponge spicules and (v) oval forms (<1 µm in diameter) with included PGM nanoparticles, similar to those observed in experiments with PGE-reducing bacteria. This study aims to deploy TEM and FIB techniques to characterize these PGM nanofibers to further asses the mobility of PGE linked to bio-weathering processes in tropical soils.

Contact person: Dr. Josep Roqué Rosell (josep.roque@ub.edu)

Title of the project: Nanoscopic origin of the anomalous pressure-dependence of the electrostatic potential of a lipid monolayer.

Name of the Group: *Statistical Physics of Nanosystems – Complex Matter Group (Faculty of Physics)*

Short description of the project: Phospholipid monolayers are model systems to study how biological membranes interact with biomolecules (e.g., proteins and cholesterol) or nanomaterials. Experiments measure their electrostatic properties, but do not clarify the nanoscopic origin of the anomalous dependence of the surface electrostatic potential with lateral pressure. We propose to study by all-atom simulations the correlation between this anomaly and the local changes in the configuration of the lipids and the hydration water. To gain further insight, we plan to explore the temperature dependence of such electrostatic properties of the membrane and compare our results with current experiments.

Tasks:
1. To reproduce by all-atom molecular dynamics simulations the experimental dependence of the electrostatic potential on the monolayer lateral pressure.
2. To identify the contributions to the electrostatic potential arising from the lipid heads, tail and the hydration water and to find the correlation between the lipids configuration and the electrostatic potential that they generate.
3. To investigate the temperature dependence of the electrostatic properties of the monolayer.

Contact persons:
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Requirements: Strong motivation, scientific curiosity, enthusiasm for exploring new phenomena with potential applications in nanomedicine.

Title of the project: Interaction of beta amiloyd fibrils with functionalized nanoparticles.

Name of the Group: *Statistical Physics of Nanosystems – Complex Matter Group (Faculty of Physics)*

Short description of the project: Functionalized nanoparticles (NPs) can interact with the β-amyloid (Aβ40) peptides and avoid their self-assembly into toxic oligomers and fibrils, which have been linked to the development of neurodegenerative diseases such as Alzheimer's disease. In collaboration with synthetic chemists, we plan to investigate how *PEGylated* gold NPs can prevent the assembly of β-amyloid proteins in solution. By using computer simulations, we will evaluate the interaction energies between β-amyloid and the functionalized NPs under different conditions, for a better design of strategies to avoid the β-amyloid fibrilization.

Tasks: By all-atom molecular dynamics simulations and standard free energy (Umbrella sampling and Metadynamics) calculations we will:
1. Characterize the interaction between Aβ40 peptides with the polymers HS-PEG2100-COOH (negatively-charged) and HS-PEG2100-OMe (non-charged) grafted to the NPs.

2. Characterize the Aβ40-Aβ40 interaction and the competition between Aβ40-Aβ40 and Aβ40-polymer interaction in experimental conditions.
3. Evaluate curvature effects in the interaction of Aβ40 with functionalized AuNPs of different sizes (5, 10 and 15nm) using a coarse-grained model built from previous results.

Contact persons:
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Dr. Carles Calero, carles.calero@ub.edu

Requirements:
Strong motivation, scientific curiosity, enthusiasm for exploring new phenomena with potential applications in nanomedicine.

Title of the project: Computational Study of Protein-Nanoparticle interactions.

Name of the Group: *Statistical Physics of Nanosystems – Complex Matter Group (Faculty of Physics)*

Short description of the project: Biomolecules in contact with nanoparticles (NPs) spontaneously adsorb and form a "protein corona". The corona composition depends on the time-dependent environmental conditions and determines the NP's fate within living organisms and its toxicity or its potential medical applications. The process of corona formation is challenging due to the large number of molecules involved and to the large span of relevant time scales ranging from 100 μs to hours. We plan to study by simulations within a multiscale approach the interactions between proteins and NPs. We will calculate the potential of mean forces mediated over different protein-NP relative orientations for silica NPs in a model plasma made of three blood proteins (human serum albumin, transferrin, and fibrinogen) which compete to adsorb on the NP surface, as tested in experiments. The calculations will allow us to develop a model for the systematic prediction and control of protein−NP corona composition based on a hierarchy of equilibrium protein binding constant.

Tasks: By adopting a model for computer simulations calibrated by experimental protein−NP binding affinities, that correctly reproduces experimental data, we will calculate:
1. The potential of mean forces of protein-protein and protein-NP interaction for NPs of different compositions (silica, metal iron oxide, lipid) in a model solution made of one of the following blood proteins: human serum albumin, transferrin, and fibrinogen
2. The protein−NP corona kinetics when the three proteins are competing for the same NP and how the prediction compare with the available experimental data.

Contact persons:
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Requirements:

Strong motivation, scientific curiosity, enthusiasm for exploring new phenomena with potential applications in nanomedicine.