Project Proposals offered at IN²UB

INDEX

NanoMet

In-Situ Characterization of resistive-switching operational devices.

Name of the Group: *Laboratory of Electron Nanoscopies (LENS) from the group MIND (Micro-nanotechnologies and Nanoscopies for Electrophotonic Devices)*

Short description of the project: An STM sample holder will be used in the TEM to probe in-situ the properties of resistive-switching operational devices

Contact: Dr. Sonia Estrade (sestrade@ub.edu);

Prof. Francesca Peiró (francesca.peiro@ub.edu)

Novel computational tools to classify EEL spectra according to ELNES

Name of the Group: *Laboratory of Electron Nanoscopies (LENS) from the group MIND (Micro-nanotechnologies and Nanoscopies for Electrophotonic Devices)*

Description: The object of this Masters Thesis is the application of novel computational tools based on artificial intelligence to the classification of electron energy loss (EEL) spectra according to ELNES; in particular, focusing on the O K edge in transition metal oxides.

Requirements: Being familiar with programming in Python

Contact: Sonia Estradé (sestrade@ub.edu)

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

Name of the Group: Statistical Physics of Bio-Nano Systems and Complex Matter

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.

Contac:

Dr. Giancarlo Franzese, gfranzese@ub.edu

Dr. Carles Calero, carles.calero@ub.edu

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

Computational Study of Protein-Nanoparticle interactions.

Name of the Group: Statistical Physics of Bio-Nano Systems and Complex Matter

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:

Dr. Giancarlo Franzese, gfranzese@ub.edu

Requirements:

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

Interaction of beta amiloyd fibrils with functionalized nanoparticles.

Name of the Group: Statistical Physics of Bio-Nano Systems and Complex Matter

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:

Dr. Giancarlo Franzese, gfranzese@ub.edu

Dr. Carles Calero, carles.calero@ub.edu

Requirements:

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

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

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)

NanoBio

Early detection of circulating tumour biomarkers in situ with implantable vascular sensor

Name of the Group: Nanobioengineering and Biomaterials Unit

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@ub.edu

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

Name of the Group: Nanobioengineering and Biomaterials Unit

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, mmir@ub.edu

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

Name of the Group: Microbial Enzymes for Industrial and Environmental Applications

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)

Patterned substrates for colocalized SPM-optical experiments on cells

Name of the group: Bioelectrical Characterization at Nanoscale

Short description of the project: The aim of this project is to obtain a multiparametric characterization of different cell properties by Scanning Probe Microscopy (SPM) and optical techniques. For this purpose, it is necessary to localize the same cell in experiments that will be performed with different equipment. The project consists in fabricating patterned and bio-compatible substrates for cell deposition, that have the characteristics of being conductive and transparent. After verification of cell deposition, SPM characterization will be performed to obtain mechanical and electrical properties on the same cell. Furthermore, confocal/optical microscopy will be added to the characterization.

Contact person: Annalisa Calò, annalisa.calo@ub.edu

Functional characterization of self-assembled nanomaterials with the SPM

Name of the group: Bioelectrical Characterization at Nanoscale

Short description of the project: Out of equilibrium self-assembled nanomaterials constitute a class of materials synthesized with new chemical routes. As they can reconfigure and adapt according to their environment, they constitute ideal materials for interfacing with cells for applications as drug delivery and detection systems. The characterization of their dynamic properties is challenging, due to the small size and the lack of characterization techniques with appropriate resolution and sensitivity in space and time. In this project, the scanning probe microscope (SPM) will be used to measure topographical, mechanical, and dielectric properties of self-assembled nanoparticles. This project has the aim to provide functional characterization to assess how properties of these nanomaterials can affect relevant parameters in biomedicine, like the toxicity or cell entry.

Contact: Dr. Annalisa Calò, annalisa.calo@ub.edu

NanoPharmaMed

Therapeutic Applications of Stimulus Triggered Delivery Systems

Name of the Group: Cellular Responses to Xenobiotics

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

Hyperthermic nanocarriers with thermo-controlled drug release properties

Group: nanoBIC

Short description of the project: The proposed PhD project is focused on carrying out thermo-release studies of cytotoxic compounds grafted to nanoparticles. It consists in designing and preparing iron-oxide nanoparticles (Fe_3O_4 NPs) decorated with thermolabile groups, which will be used to release a drug and/or an imaging agent (therapy, diagnosis or theranostics). The main idea is to use the remarkable properties of Fe_3O_4 nanoparticles, like for instance their ability to cross the blood-brain barrier or/and magnetism, to produce efficient drug nanocarriers. Hence, Fe_3O_4 NPs will be generated, which will contain specific functional groups aimed at detecting (diagnosis) or/and treating (therapy) cancer. The potential drug or fluorescent molecule will be connected to the NPs through thermolabile groups. The release of the bioactive compound will be achieved through hyperthermia, applying an alternating magnetic field. The heat generated will give rise to a cyclization reaction of the thermosensitive group that will result in a bond cleavage and subsequent liberation of the drug/prodrug or fluorescent agent.

Contact person: Dr. Patrick Gamez, patrick.gamez@ub.edu

Metal nanoparticles for controlled delivery of DNA

Name of the Group: nanoBIC

Short description of the project: Gene therapy may allow to treat a disease by inserting a genetic material (*e.g*. DNA, siRNA) into a patient's cells, followed by expression and production of a deficient protein; this avoids the use of drugs or surgery. However, a successful delivery of genetic material is limited by their large size, vulnerability against enzymatic degradation and anionic nature. Such features make gene delivery very challenging. Therefore, carriers are commonly required to enhance their entry into cells/tissues.

This project aims at using functionalized metal nanoparticles as carriers for controlled delivery of DNA. To do so, the student will optimize the size and surface functionalization of metal nanoparticles to immobilize and stabilize different structures of DNA, which will be released afterwards upon an external stimulus.

The student will be trained in nanoparticle synthesis and functionalization, and in a wide range of instrumental techniques covering the characterization of nanomaterials and biophysical studies of DNA-nanoparticle interactions.

PhD studies in a similar o related topic will be encouraged in our group for talented students.

Contact person: Dr. Ana Belén Caballero Hernández, ana.caballero@ub.edu

Delivery of Iridium-Based Photosensitizers using Gold Nanoparticles for Photodynamic Therapy of Cancer

Name of the Group: nanoBIC

Short description of the project: This project aims at using gold nanoparticles as carriers for an enhanced delivery of antitumor, photosensitizing iridium compounds. To do so, the student will optimize the surface functionalization of gold nanoparticles to carry a series of Ir(III) compounds. Afterwards, photodynamic activity will be evaluated and the nanoconjugates will be tested using several tumor cell lines.

The student will be trained in nanoparticle synthesis, functionalization, and characterization of nanomaterials. Also, the student will receive basic training in cell culture from cell biologists. PhD studies in related topics will be encouraged in our group for talented students.

Contact: Dr. Ana Belén Caballero Hernández, ana.caballero@ub.edu.

Hybrid nanomaterials with enhanced singlet oxygen generation for photodynamic therapy

Name of the Group: *Supramolecular Systems in Nanobiomedicine*

Short description of the project: Photodynamic therapy (PDT) is a therapeutical strategy for cancer, where photosensitizer drugs (PS) are administered, and then activated with focalized light to produce singlet oxygen (SO) in the tumour, inducing the death of cancer cells. However, PS are distributed across the body, leading to important side effects after sun exposure. Incorporation of PS onto nanostructured materials will improve their safety and efficacy. Preliminary work indicates that encapsulation or conjugation of PS in the materials enhances their capability of generating SO and the overall efficiency of the PDT process. This project will involve the preparation of different PS and their immobilization onto water soluble nano and microparticles functionalized with specific antibodies as deliverers to cancer cells. Assessment of their potential in PDT will be done by analysis of singlet oxygen production. There is the possibility of continuity towards a doctoral thesis.

Contact: Prof. Ma Lluïsa Pérez-García, mlperez@ub.edu

Light-controlled molecular machines

Name of the Group: Supramolecular Systems in Nanobiomedicine (Faculty of Pharmacy)

Short description of the project: Artificial molecular motors, where molecules can travel across microscopic materials in the presence of an external stimulus, have great implications in many aspects of science. However, a controlled transport of molecules across supramolecular systems has yet to be achieved. Based on preliminary experiments, we intend to design a purely supramolecular system where a molecular “traveller” moves along a “path” over several microns when irradiated with visible light. Real time imaging of the motion using total internal reflection fluorescence microscopy will be used to observe molecules move along fibres upon irradiation. There is the possibility of continuity towards a doctoral thesis.

Contact: Prof. Ma Lluïsa Pérez-García, mlperez@ub.edu

Biofunctionalisation of silicon microchips for real-time intracellular sensing

Name of the Group: Supramolecular Systems in Nanobiomedicine (Faculty of Pharmacy)

Short description of the project: The present project will involve the bio-functionalisation of silicon microparticles with synthetic organic moieties designed to interact with biological material and sense its function. The overall objective is to prepare cellular sensors to monitor different cellular parameters, such as the presence of different peptides and proteins involved in apoptosis with implications in cancer. In order to succeed in this complex project a highly interdisciplinary approach is necessary, and the research is integrated within a coordinated project that aims to find functional microchips to study, tag and act on living cells. There is the possibility of continuity towards a doctoral thesis.

Contact: Prof. Ma Lluïsa Pérez-García, mlperez@ub.edu

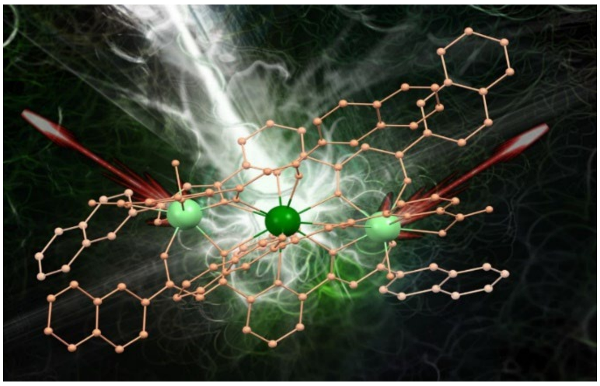
NanoMagnetics

Novel Heterometallic Lanthanide Molecules for Quantum Technologies or exòtic Photoluminescence.

Name of the Group: LabMolDesign (Faculty of Chemistry)

Short description of the project: Did you know that the compounds you will make may be the qubits and quantum gates of future quantum information technologies (QIS)? At the LabMolDesign, we have discovered a method to prepare selectively heterometallic lanthanide coordination molecules that are relevant for QIS and also to unveil novel photoluminescent properties. You will prepare these compounds and have hands-on experience of characterization (powder or single crystal X-ray diffraction in our lab or at ALBA synchrotron, paramagnetic NMR, magnetometry, EPR, etc.).

Contact: Prof. Guillem Aromí (aromi@ub.edu)

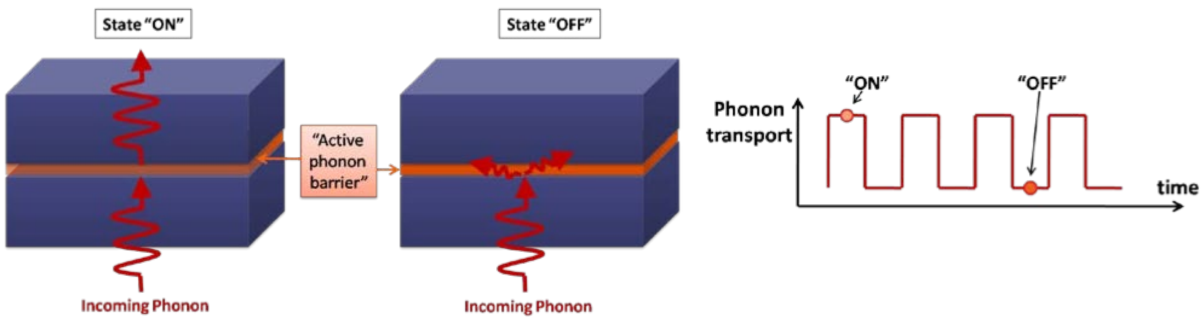


Electric and magnetic control of phonon transport

Research groups: Group of Magnetic Nanomaterials

Description of the project:

Many of the major technological breakthroughs occurring in the last few decades rely on our effective capability to control and manipulate two elementary particles: electrons (both charge and spin) and photons. In particular, they are responsible for the current semiconductor technology, information storage devices, wireless communication, optical fibers, etc. In the rapid pace of these technological advancements, phonons, quasiparticles accounting for elementary vibration modes of the lattice, have lagged far behind, relegated to second place, mainly because of the difficulty in manipulating them. However, if similar degree of control over phonons—such as the technology-readiness over electrons—were possible, a radically new range of applications and research directions could be unfolded. First, since phonons are the main heat carriers in solids, their control would allow channeling the heat flow—and, thus, the thermal energy—at will, propelling new possibilities for thermal energy management and harvesting. Second, it might build up a completely new technology for logic, data storage devices and computing mechanisms utilizing phonons: the so-called phononics.



The main objective of the project is the realization of functional solid-state phononic devices such as an active phonon barrier depicted in the figure above that could reversibly allow (state ON) or inhibit (state OFF) the phonon propagation using an external stimulus (an electric field, for instance). Moreover, the two phononic states (ON/OFF) should be robust and stable once the external stimulus is removed in order to make viable a binary code using phonons.

Contact: Eric Langenberg (eric.langenberg@ub.edu), Xavier Batlle (xavierbatlle@ub.edu)

Enhanced plasmonic properties in arrays of multifunctional nanostructures

Research groups: Group of Magnetic Nanomaterials

Research on:

– Optical response of ordered plasmonic nanostructures manufactured by electron beam lithography or nanoimprinting

– Perfect optical absorbers in the visible and near-infrared

– Experiments and numerical simulations

– Highly-sensitive sensor platforms

– Chiral molecular recognition

– Magnetoplasmonics

Contact: Arantxa Fraile Rodríguez (arantxa.fraile@ub.edu)
Xavier Batlle (xavierbatlle@ub.edu)
Amílcar Labarta (amilcar.labarta@ub.edu)

Quantum materials and devices

Name of the Group: Magnetism

Description of the project: Description of the project: Two-dimensional (2D) van der Waals quantum materials hold great promise to revolutionize the scientific and technological fields. The immense interest in this research area is also evident by two recent Physics Nobel laureates, for the discovery of graphene in 2010 and for the theoretical explanations of the topological phases of matter in 2016. The TFM student will learn fabrication and measurements techniques of devices based on 2D quantum materials. Possibility to continue in the PhD program after the TFM.

Contact: Dr. Marius Costache (costache@ub.edu)

2D materials: metallic / molecular heterostructures for spintronic applications

Group: Molecular Nanoscience Laboratory

Project: In this project the candidate will prepare surface deposited nanomagnets on various surfaces (functionalized Silicon, MgO or Kapton/Au). To prepare hybrid heterostructures, Au, Co or permalloy will be deposited using sputtering on top of the nanomagnet layer. The main goals are to establish the robustness of the nanomagnet layer will be studied, and the magnetic properties of the prepared heterostructures. This project is suitable for the Master of Nanoscience and for the Master of Applied Materials Chemistry.

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

Synthesis of functional molecules for spintronic applications

Group: Molecular Nanoscience Laboratory

Project: In this project the candidate will focus on the synthesis of new nanomagnets amenable to surface deposition. Surface deposition is a requisite for the use of molecules in spintronics, quantum computing or other applications like information storage. Ligand design and molecule geometry are key factors that can be controlled by chemical synthesis. This project is suitable for the Master of Nanoscience and for the Master of Applied Materials Chemistry.

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

Bi-magnetic core@shell nanoparticles for room temperature magnetic properties modulation

Group: Laboratory of Nanostructured and Nanocomposite Materials (LM2N)

Short description of the project: Ferrimagnetic@antiferromagnetic core@shell oxide-based nanopartciles will be synthesized by means of thermal decomposition route (colloidal synthesis). This project aims at modulating the ferrimagnetic properties at room temperature through the effect of the proximity of the antiferromagnetic counterpart. This property is currently used within the heading reads based on the Giant Magnetoresistance effect. This project involves chemical synthesis and structural and magnetic characterization.

Contact: Dr. Marta Estrader martaestrader@ub.edu

Merging spin crossover materials with magnetic nanoparticles: Searching for synergistic properties

Group: Laboratory of Nanostructured and Nanocomposite Materials (LM2N)

Short description of the project: In this project, spin crossover complexes will be grown onto the surface of inorganic nanoparticles through chemical synthesis approaches. The optical, magnetic and thermal properties of the inorganic nanoparticle will be entangled with the spin crossover effect seeking for interconnected changes of their respective properties. This project comprises chemical synthesis and structural and magnetic characterization.

Contact: Dr. Marta Estrader martaestrader@ub.edu

NanoPhotoElectro

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:

Dr. Blas Garrido Fernández, bgarrido@el.ub.edu

Dr. Sergi Hernández Márquez, shernandez@ub.edu

Simulation of photonic crystals based on silicon nanopillars

Name of the Group: *MIND - Nanosystems*

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: Prof. Albert Romano-Rodriguez (albert.romano@ub.edu)

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: Prof. Albert Romano-Rodriguez (albert.romano@ub.edu)

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.

Contact:

Dr. Blas Garrido Fernández, bgarrido@el.ub.edu

Dr. Daniel Navarro Urríos, dnavarro@ub.edu

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:

Dr. Blas Garrido Fernández, bgarrido@el.ub.edu

Dr. Sergi Hernández Márquez, shernandez@ub.edu

Inkjet Printing of metal-oxide electronic devices

Name of the Group: Systems for Instrumentation & Communicacions

Short description of the project: The aim of this project is to design, fabricate and characterize some electronic devices such as díodes, thin-film transistors, light emitting díodes or photodetectors. The main fabrication technique will be inkjet printing, a cheap, versatile, safe and sustainable direct-write technology useful for a variety of materials. Among the oxide semiconductors compatible with it, ZnO will be preferred, but other alloys such as ITO, SnO2, etc. are not excluded.

Contact: Dr. Anna Vilà, anna.vila@ub.edu

Green ZnO inks for inkjet printing

Name of the Group: Systems for Instrumentation & Communicacions

Short description of the project: ZnO is the metal oxide most used in printed electronics. However, many of the mixtures used in the printing ink are hazardous and can cause danger for their users. This project intends to investigate alternative inks non-hazardous, non-toxic, ecolologic and bio-compatible to inkjet print ZnO. Extrapolation to other metal oxides will be considered.

Contact: Anna Vilà, anna.vila@ub.edu

NanosMat

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

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.

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Nanomaterials for photocatalytic applications

Name of the Group: *Group ENPHOCAMAT: ENergy, PHOtonics & CAtalisys MATerials*

Short description of the project: This project is based on the development of advanced nanomaterials that hold the key to open a new generation of products for clean, renewable and sustainable energy. These breakthroughs will be reached through the control of material properties and understanding of mechanisms and phenomena at the nanoscale and atomic level. The main challenges are to understand how to get new materials capable to obtain fuels such as hydrogen and carbon reduced forms based (i.e. methane, methanol) from the carbon dioxide re-utilization at low-cost and high-efficiency. The high efficiency solar to fuel energy conversion require features that must guarantee the device functionality: i) photon absorption, ii) charge separation and carrier current management, and iii) charge transfer involving catalyst for the expected chemical transformation.

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Nanomaterials for piezoelectric energy harvesting

Name of the Group: *Group ENPHOCAMAT: ENergy, PHOtonics & CAtalisys MATerials*

Short description of the project: This project is based on the development of advanced nanomaterials that hold the key to open a new generation of products for clean, renewable and sustainable energy. These breakthroughs will be reached through the control of material properties and understanding of mechanisms and phenomena at the nanoscale and atomic level. The growth of nanostructures by hydrothermal method for piezoelectric applications will be demonstrated by using piezoresponse atomic force microscope (PFM) and with the support of a piezoelectric test device. This low-cost and fast selective-area synthesis of nanomaterials paves the way to new promising applications, such as bioelectronic applications, energy generation or self-powered sensing.

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Photoluminescence properties of ZnO/graphene nanomaterials

Name of the Group: *Group ENPHOCAMAT: ENergy, PHOtonics & CAtalisys MATerials*

Short description of the project: This project is based on the development of advanced nanomaterials that hold the key to open a new generation of products for clean, renewable and sustainable energy. Photoluminescent ZnO/Graphene nanomaterials are an emerging class of nanomaterials with unique optical properties. They each, ZnO and carbon nanomaterials, have an advantage of being nontoxic and environmentally friendly. Moreover, ZnO presents photoluminescence emission in the UV and visible region depending on the synthesis routes, shape, size, deep level, and surface defects. When combined with carbon nanomaterials,modification of surface defects in ZnO allows tuning of these photoluminescence properties to produce, for example, white light.

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Preparation and, inclusion and redox properties of mixed-valence, water soluble, Prussian Blue Analogues (PBAs).

Name of the Group: Mecanismes de reacció (MEC).

Description of the project: The construction and characteristics of water soluble and chemically resistant cyanido bridged Co^{III}/Fe^{II} cubes will be studied. The assembly reaction will be carried out by a redox-substitution mechanistically driven process from $[Fe(CN)6]^{4-}$ and [CoLCl3] where L represents a tridentate N3 or S3 ligand. The resulting mixed-valence species should present interesting intervalence character and redox properties. Furthermore, as most PBAs, the new cubes are bound to show selective alkaline cation encapsulating properties. Tuning the nature of the tridentate ligand from N3 to S3 should produce an enhanced stability of the magnetically active Co^{II}/Fe^{III} isomer, thus allowing the study of new electron-transfer processes.

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Study of the luminescent properties of Gold Nanoparticles functionalized with coumarin ligands.

Name of the Group: Supra and Nanostructured Systems, SuNS

Short description of the project: Metal and semiconductor nanoparticles present interesting properties depending on their size and shape. The combination of these properties with the introduction of new groups at the surface of the nanoparticles can produce hybrid materials with new and interesting properties and functions. One example is the use of gold nanoparticles as sensors in light-harvesting systems or as modulators of the fluorescent properties of dyes immobilized in their surface. In this project, we will develop gold nanoparticles functionalized with dyes (coumarine ligands) to obtain new photoluminescent materials that could be use in the field of molecular recognition. PhD studies are possible after the master thesis.

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Phosphorescent organometallic materials as ideal candidates for OLEDs or biomedicine.

Name of the Group: Supra and Nanostructured Systems, SuNS

Short description of the Project: The synthesis of organometallic Au(I) or Pt(II) complexes with potentially outstanding luminescence properties will be carried out. In this project, the master Student will perform organic and organometallic synthesis. Especial attention will be paid to the characterization of the emissive properties of the complexes and their precursors in order to select good candidates for biomedical applications and as OLEDs. PhD studies are possible after the master thesis.

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Hybrid Inorganic Nanoparticles As Bimodal Therapeutic Agents

Name of the Group: Laboratory of Nanostructured and Nanocomposite Materials, LM2N

Short description of the project: Nanotechnology is gaining an increasing role in the therapy and diagnosis fields. In this Master thesis the synthesis and characterization of new nanostructured bimodal therapeutic agents is pursued through the design of appropriate inorganic hybrid nanoparticles. This goal will be achieved by the presence of both a magnetic and a semiconductor domain sharing an interface within the nanoparticle. Each of the domains would accomplish its therapeutic role under the effect of a specific external stimulus such as light or magnetic field. Colloidal synthetic strategies will be used for the synthesis of these size and shape controlled hybrid nanoparticles, and a wide variety of structural, morphological, chemical and physical characterization techniques will be employed to assess the suitability of the samples obtained.

Contact:

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Investigation of organic light emitting devices (OLEDs) for blue and white emission

Name of The Group: Organic Materials

Proposal: Study of new organic blue-luminescent materials. Spin coating and vacuum deposition will be considered for the preparation of their thin films for emission measurements. The study will include the analysis of different hosts and their effect in the quantum yield and in the efficiency of the organic light emitting devices fabricated.

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Synthesis and study of carbazole-based azochromophores for controlling the order in the solid State. Application to organic thin-film transistors TFTs.

Name of The Group: Organic Materials

Proposal: In this master thesis the student will fabricate and characterize organic devices. In particular, thin-film transistors will be fabricated using small-molecules as organic semiconductors or organic dielèctric, whose geometry and properties could be modified by light. The electrical performance of the devices will be determined and correlated with the structural and optical properties of the organic molècules. X-Ray and AFM techniques will be used for their characterization.

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Metal carbides nanocompounds/ 3D graphene nanostructures for electrocatalytic hydrogen production.

Name of the Group: Group *ENPHOCAMAT*: ENergy, PHOtonics & CAtalisys MATerials

Short description of the project: Hydrogen is a renewable energy carrier which holds great promise for wide use in a post fossil fuel economy. To accelerate its adaptation in industrial scale, novel electrolyzers are required, which will promote hydrogen production through water splitting. The proposed project aims on the preparation of nanocompounds based on transition metals and 3D graphene nanostructures, which are expected to show an enhanced performance when used as cathode electrodes in electrocatalytic water splitting. The selected student is expected to work on the preparation of the compounds, combining plasma enhanced chemical vapor deposition and magnetron sputtering technologies, as well as study the performance of the above compounds in water electrolysis.

Further reading:

1] S. Chaitoglou, T. Giannakopoulou, G. Papanastasiou, D. Tsoutsou, A. Vavouliotis, C. Trapalis, A. Dimoulas *Cu vapor-assisted formation of nanostructured Mo2C electrocatalysts via direct chemical conversion of Mo surface for efficient hydrogen evolution reaction applications* Applied Surface Science 510 (2020) 145516

2] Yasmín Esqueda-Barrón, Angel Pérez del Pino, Pablo García Lebiere, Arevik Musheghyan-Avetisyan,̀ Enric Bertran-Serra, Enikö György, and Constantin Logofatu *Boost of Charge Storage Performance of Graphene Nanowall Electrodes by Laser-Induced Crystallization of Metal Oxide Nanostructures* ACS Appl. Mater. Interfaces 2021, 13, 17957−17970

Contact: Dr. Stefanos Chaitoglou, stefanoschaitoglou@ub.edu, Dr. Enric Bertran, ebertran@ub.edu

New organometallic precursors for selective hydroacylation reactions

Name of the Group: Homogeneous Catalysis

Short description of the project: The hydroacylation reaction can be defined as the coupling between an aldehyde and an alkene or alkyne, usually catalyzed by Rh(I) precursors. Given the immense number of aldehydes and unsaturated compounds available, it is a reaction with extraordinary potential for the synthesis of molecules of interest but despite this, it has been poorly developed. The Homogeneous Catalysis group has recently been working on the synthesis of P-stereogenic methylene bridge diphosphanes, which have been applied to reduction reactions of functionalized olefins and ketones (Dalton Trans. 2023, 52, 2424-2439). This proposal aims to use this expertise to prepare certain diphosphanes that have been specifically designed, considering literature precedent, for selective hydroacylation reactions. Their coordination towards organometallic Rh(I) moieties will be explored and the complexes obtained will be studied as catalytic precursors in hydroacylations.

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Compositionally-controlled multinary Bi-based nanocrystals for energy conversion technologies.

Group: Laboratory of Nanostructured and Nanocomposite Materials (LM2N)

Project: The use of semiconductor nanocrystals with quantum properties in energy conversion technologies has attracted a great interest in the recent years. The use of ternary or quaternary semiconductors offers a new way to control physical properties by means of chemical composition tuning. This Master thesis is dedicated to the development of new colloidal bottom-up synthetic strategies for the preparation of size and shape-controlled semiconductor nanocrystals made by at least three different elements in an attempt to improve the performance of future optoelectronic and thermoelectric devices.
Contact Person: Dr. Albert Figuerola (albert.figuerola@ub.edu)

Colloidal growth of Ag-based chalcohalide nanocrystals as alternative and highly absorbing materials for photovoltaic technologies.

Group: Laboratory of Nanostructured and Nanocomposite Materials (LM2N)
Project: Silver chalcohalides are an emerging family of inorganic semiconductors that are commonly denoted as Ag3XY, where X and Y stand for chalcogen and halogen anions, respectively. Despite their promising chemical, structural and optical properties of its bulk form, very few studies have been undertaken in order to control their synthesis at the nanoscale and explore the new properties thereof derived. This Master thesis is dedicated to the development of new colloidal bottom-up synthetic strategies for the preparation of size and shape-controlled silver chalcohalide semiconductor nanocrystals, in order to make a step forward in the fabrication of efficient, sustainable and environmentally friendly photovoltaic devices.
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Hot Spot engineering in plasmonic nanostructures for photothermal therapy.

Group: Laboratory of Nanostructured and Nanocomposite Materials (LM2N)
Project: Localized Surface Plasmon Resonance occurs when the size of nanostructures is much shorter than the wavelength of the excitation light. It is an optical absorption phenomenon that takes place in certain metal and semiconductor nanostructures. The plasmon induces the confinement of incident optical energy, producing high electromagnetic field enhancements, which might be of special interest in the development of surface-enhanced Raman spectroscopy (SERS)-based sensors. This Master thesis is dedicated to the development of new colloidal bottom-up synthetic strategies for the preparation of size and shape-controlled

plasmonic nanocrystals, together with their morphological, chemical and optical characterization.

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Transversal Proposals

Iron oxide nanoparticles for targeted cancer therapy

Name of the Groups: Cancer therapy group and Molecular Nanoscience Laboratory

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.

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Rh, Ir, and Re complexes with pyrenylphosphanes as chemotherapeutic agents

Name of the Group: Homogeneous Catalysis and nanoBIC

Short description of the project: the proposed project aims to develop several types of Rh(III), Ir(III), and Re(0) complexes with pyrenylphosphanes, following our previous results (Inorg. Chem. 2021, 60, 7974-7990), which showed very promising antineoplastic activities of the same kind of ligands coordinated Ru(II)- and Os(II)-arene moieties. We have demonstrated that pyrenylphosphanes show a remarkable cyclometallating ability, which results in high cytotoxicities. The prospects of expanding this chemistry to other metals is very exciting and should lead to very active systems.

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Superhyperfine coupling for qubit/qudit performance

Name of the Group: Molecular Magnetism and Homogeneous Catalysis

Short description of the project: the use of hyperfine coupling to create electronuclear states which help in the control of the nuclear transitions has been studied in the past few years. The main idea is to use the electronic spin S = ½ as an ancilla for its own nucleus in an atom. This method has demonstrated to be successful and very good coherence times with low error rates have been achieved. The present project goes one step beyond and proposes to use the superhyperfine coupling (the hyperfine coupling in between two different atoms) to prepare the electronuclear states. In this way, thanks to the synthetic power of chemistry inspired by a creative design, the distance in between two different atoms will be easily controlled. The use of organic ligands containing different types of P-donors and its coordination to metallic cations with low valences, electronic spin ½ and different nuclear spins, will help us to understand how superhyperfine coupling could help in scaling up of the building blocks for quantum computing and quantum sensing.

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Metal organic frameworks (MOF) for catalysis and chemical sensing

Name of the Group: Homogeneous Catalysis (Faculty of Chemistry) and Micro and Nanotechnology and nanoscopies for Electronic and Electrophotonic Devices (Faculty of Physics)

Short description of the project: organic catecholates are planar ligands that have been used for the preparation of crystalline two-dimensional conjugated porous extended frameworks (2D-cMOFs) by employing square-planar metal complexes. These 2D-cMOFs have intrinsic conductivity, porosity, and luminescence. The aim of the present work is to prepare and characterize new metal-catecholates and chemoresistive gas sensors and to check their selectivity and sensibility sensing volatile organic compounds (VOCs) and in catalytic processes like Suzuki-Miyaura and Heck-Cassar-Sonogashira Cross coupling.

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Monitoring climate change gases with sensors based on 2D materials

Name of the Group: Homogeneous Catalysis (Faculty of Chemistry) and Micro and Nanotechnology and nanoscopies for Electronic and Electrophotonic Devices (Faculty of Physics)

Short description of the project: the overall objective is to develop a novel platform in which an array of sensing devices of climate change gases based on 2D materials (such as MoS_2 and WS_2) are integrated. We will develop the hybridisation of the surface of the 2D materials to make them more sensitive to specific target gases. The initial ideas are addition of metal and/or metal oxide nanoparticles, such as Ag, Au, Pd, SnO_2, TiO_2 and ZnO, which will provide gas detection specificity and an amplified response, but we will explore several different synthetic approaches reported successfully in literature such as electrodeposition, or sol-gel methods.

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Design and Evaluation of Small Iron Oxide Nanorods in Cancer Preclinical Assays

Name of the Group: nanoBIC and Group of Magnetic Nanomaterials

Short description of the Project: Cancer is a major public health and economic issue, and its burden is set to spiral. In the last five years, anisotropic Iron oxide nanorods (IONRs) have gained major importance as agents for combination therapy to exceed the efficiency of various anti-cancer drugs. IONRs offer advantages such as increased magneto-mechanical torque for improved magnetic hyperthermia and magnetic resonance imaging responses, and a larger surface area for efficient ligand attachment, facilitating cell interaction and drug release. Indeed, an interesting approach to ensure the biocompatibility of these systems is to coat them with a protein corona of a natural product such as Bovine Serum Albumin (BSA). This protein can form a protective layer, improving colloidal stability and biocompatibility in biological media, while drug conjugation and release can occur naturally by tunning the pH. Despite the intensive research in the field, comprehensive research is needed to assess cytotoxicity based on particle characteristics such as size, shape, and surface functionalization. The objective of this project is to advance the field by perfecting the design of small IONRs at all levels, including morphology, composition, surface coating, and specific drug conjugation for their biological evaluation in prostate and breast cancer cells.

Planned tasks:

Task 1: Optimize our synthesis method for Small IONRs, tailoring their dimensions and magnetic characteristics.

Task 2: Functionalize the resulting IONRs with BSA to enhance their biocompatibility and ensure their stability in water solutions.

Task 3: Explore the stability of the IONRs when they are exposed to biological environments, preserving their structural integrity and functionality.

Task 4: Assess how well the IONRs, once synthesized, coated, and stabilized, can serve as carriers for targeted drug delivery in cancer treatment.

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