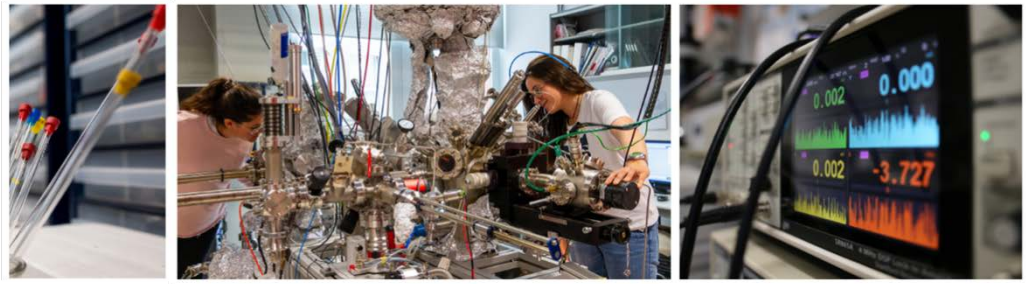

MASTER THESIS OFFER 2020/2021

1 **Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications**

2 **New Photoactivated Synthesis Routes to Single-Chain Nanoparticles**

3 **Surveying chemical reactions at surfaces and interfaces properties**

4 **Physics and Chemistry of Curved Crystal Surfaces: oxygen, carbon monoxide and carbon dioxide chemisorption and dissociation on stepped surfaces**

5 **Cyclic polymers for biomedical application**

6 **High frequency phenomena in soft magnetic nanostructured materials**

7 **Nanostructured materials for artificial photosynthesis**

8 **Dimerized diamond chain in magnetic fields**

9 **Optical properties of 2D materials with ab-initio methods**

10 **Stacking of Two-dimensional Graphene-like Materials**

11 **Anharmonic effects on the nuclei wave functions**

12 **Anisotropic phonon polaritons in biaxial van der Waals materials**

13 **Theory of optical nanocavity-molecule interaction**

14 **Ultrafast adsorbate vibrational dynamics**

15 **Quantum transport and spin physics in graphene nanostructures**

16 **The Dzyaloshinskii-Moriya Interaction in ultrathin films**

17 **Hybrid perovskites for photovoltaics – stability and degradation mechanisms**

18 **Exploring the growth and the electronic structure of in-plane heterostructures of transition metal dichalcogenides**

19 **Molecular dynamics study of Calmodulin**

Updated on 24/09/2020

1 Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications

Single-chain nanoparticles (SCNPs) are the result of applying single-chain technology to individual polymer chains, giving rise to versatile folded/collapsed soft nano-objects of ultra-small size (2-20 nm). Significant effort has been spent in last years to endow SCNPs with useful and bioinspired applications for the fields of nanomedicine, bioimaging, biosensing, protein mimicry and catalysis, among others. This Master Thesis project is aimed to produce SCNPs with fluorescent properties of great interest for sensing and bioimaging applications.

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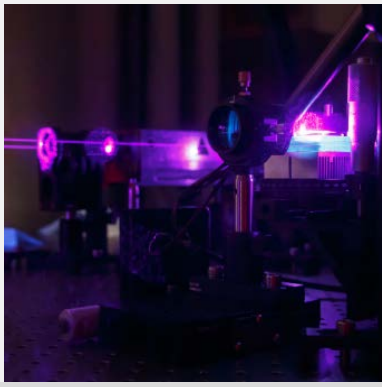
2 New Photoactivated Synthesis Routes to Single-Chain Nanoparticles



Single-chain nanoparticles (SCNPs) are the result of applying single-chain technology to individual polymer chains, giving rise to versatile folded/collapsed soft nano-objects of ultra-small size (2-20 nm). Significant effort has been spent in last years to endow SCNPs with useful and bioinspired applications for the fields of nanomedicine, bioimaging, biosensing, protein mimicry and catalysis, among others. This Master Thesis project is aimed to explore new, facile UV irradiation-based synthesis routes to SCNPs.

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3 Surveying chemical reactions at surfaces and interfaces properties

The growing interest for organic-based materials derives from their potential in functional platforms for electrochemical energy conversion and storage system. This attractive potential emerges from the capability to form tunable, ordered and periodic structures with shape or chemical composition defined by the choice of molecular precursors. Yet, the material efficiency, its reactivity and charge transport are still challenging. Thus, reaching device applications requires a better understanding of the materials and interfaces at fundamental level. The present project addresses experimental questions at the joint frontier between surface physics and chemistry concerning the synthesis and characterization of organic interfaces. Here, we aim to clarify the fundamental aspects of metal-organic surface, such as the chemical reactions leading to molecular reactivity on surfaces, their electronic structure and stability towards charge storage/transfer and/or capability to promote catalysis. The characterization of these will be performed in ultra-high-vacuum using scanning probe techniques (STM, STS, AFM) at 1-Kelvin. These techniques will allow improving our knowledge on the synthesis of efficient organic layer for applications.

The candidate will acquire various skills, as handling ultra-high-vacuum techniques and sample preparation, dealing with cryogenic temperatures (liquid nitrogen/helium), state of the art scanning-probe techniques, physical-chemical approaches of surface science.

+ INFO

https://cfm.ehu.es/atomic-spectroscopy

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4 Physics and Chemistry of Curved Crystal Surfaces: oxygen, carbon monoxide and carbon dioxide chemisorption and dissociation on stepped surfaces

Chemisorption and dissociation of gas-phase reactants are fundamental to understand heterogeneous catalysis. By exposing curved crystals of Pt, Pd, Cu, Ni, and Rh to O2, CO and NO we investigate the role of active step sites during gas-metal interactions for the most relevant catalytic processes, namely CO and NO oxidation. The work combines Valence Band and Core-level photoemission spectroscopy, and also implies the use of other Surface Science Techniques, namely LEED and STM and ARPES, all operating in Ultra-High Vacuum conditions.

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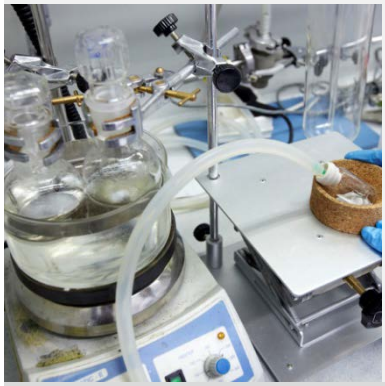
5 Cyclic polymers for biomedical applications

Cyclic polymers possess unique physico-chemical properties compared to their linear counterparts as a result of the absence of end-groups. In the past 60 years, examples of cyclic biomacromolecules have been found in nature, being circular DNA the first cyclic polymer to be studied in detail. The impact of these findings combined with the development of new synthetic tools has provided an increased motivation to further explore the synthesis, physical characterization and potential applications of cyclic polymers.

The aim of this Master Thesis is the synthesis of materials based on cyclic polyethers with potential biomedical applications, either in photodynamic therapy or drug release. The student will learn state-of-the art techniques for synthesizing and characterizing polymers with complex structures (MALDI-TOF MS, GPC with triple detection, NMR, FTIR, Raman spectroscopy, etc).



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6 High frequency phenomena in soft magnetic nanostructured materials

Phenomena like giant magnetoimpedance effect (GMI) and ferromagnetic resonance (FMR) in different families of soft magnetic amorphous, nanocrystalline and nanogranular metallic alloys have open new opportunities of research owing to the promising and, even, real technological applications. Such scientific research has dealt with several aspects concerning the intrinsic magnetotransport properties (i.e.: frequency range, intensity of the effect, magnetic field to observe possible maximum, noise…) as well as those related with microstructural (mainly amorphous or nanocrystalline) or geometrical character (wire, but these phenomena have been reported in glass-coated microwire, ribbon, multilayers, lantanide compounds and, therefore, high frequency magnetotransport phenomena are actually opening a new branch of research in soft magnetic materials. GMI and FMR combine the micromagnetics of soft magnets with the classical electrodynamics. Obviously, the different geometry and sample dimension together with the magnetic anisotropy lead to some differences in the GMI response like the range of frequency and the magnetic field dependence of the impedance curve with one or two peaks or even, it could be relevant the shape of the peak, etc.

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7 Nanostructured materials for artificial photosynthesis

The control over the materials structure down to nanoscale as well as their electronic structure are the most important requisites to develop artificial photosynthetic systems that through photocatalytic conversion can efficiently store light energy in chemical bonds. Especially important is the nanomaterials composition that defines light harvesting capacity and drive catalytic reactions via electron transfer. The aim of this project is the rational design and development of a hybrid nanoparticle-based photocatalyst using variety of sub-units such as molecules, supra-molecular complexes, plasmonic nanoparticles and quantum dots to be later assessed on a single particle level with sub-particle resolution. The project is multi- disciplinary and involves a variety of techniques, ranging from fabrication of nanostructures to their characterization using absorption, photoluminescence and Raman spectroscopy, fluorescence confocal lifetime microscopy imaging as well as fluorescence correlation spectroscopy. The material development and advanced characterization techniques will serve to study the fundamentals of photocatalytic processes related to photosynthesis with special focus on cofactor regeneration.

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8 Dimerized diamond chain in magnetic fields

In this project, we will investigate the property of a dimerised diamond chain [1] closed on a loop geometry. We will examine the effect of an Aharonov-Bohm and transverse magnetic fluxes. The project is composed of two parts: in the first part of the project, we will investigate the spectral properties of the system as a function of the two fluxes, the dimerisation geometry and the length of the chain. From the spectral properties, we will also analyse the persistent current induced by the Aharonov-Bohm flux [2]. In the second part of the project, we will investigate a possible implementation of the investigated set-up in the framework of photonic lattices using optical induction in photorefractive crystals [3].

References:

[1] D. Bercioux, O. Dutta, and E. Rico, Ann. Phys. (Berl.) 529, 1600262 (2017)
[2] M. Filippone, C.-E. Bardyn, and T. Giamarchi, Phys. Rev. B 97, 201408 (2018)
[3] L. Tang et al., Nanophotonics (2020) https://doi.org/10.1515/nanoph-2020-0043

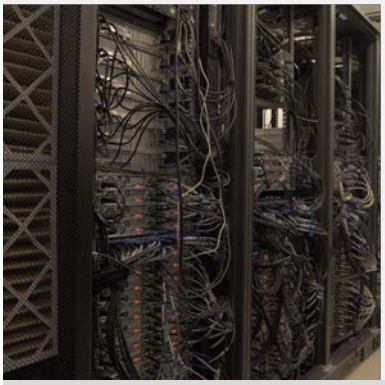
Contact: **Dario Bercioux** dario.bercioux@dipc.org

9 Optical properties of 2D materials with ab-initio methods

The investigation of the properties of 2-dimensional materials boomed after the isolation of graphene a few years ago. Many of these materials are exfoliated from a layered bulk, where the layers hold together through weak van der Walls forces. These amazing systems have promised a wide range of technological revolutions in the world of nanoscale electronics, mainly due to the ease with which their properties can be manipulated and tailored for particular tasks.

In this project, we will investigate, through numerical methods, the optical properties of some of these newly found 2-dimensional materials, with particular focus to Cu-Se based systems but potentially looking also at Sn-Se and Ag-Se structures. These materials show experimentally interesting properties for their use as optical devices in particular for light detection, manipulation, and conversion, but their electronic properties can still hide interesting new behaviours.

The student should be at ease with the use of computers, but they will gain expertise on the numerical tools during this research.



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10 Stacking of Two-dimensional Graphene-like Materials

New phenomena in condensed matter physics are based on two-dimensional materials. Although a single graphene looks promising for the future, research is today focusing on stacking several two-dimensional materials to form nanostructured materials made of carbon and other materials. The possibility to exfoliate materials and the existence of accurate experimental techniques to study single-layer materials supposed a big boost to study other layered materials. Currently much work is devoted to understand the recent finding of superconductivity in bilayer graphene. The aim of this project is to study the structural and electronic properties when having several layers of graphene either independently or sandwiched with other two-dimensional materials. During the master thesis project, the candidate will acquire knowledge in 2D materials, and gain expertise in using numerical tools, such as first-principles simulations or tight binding calculations.

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11 Anharmonic effects on the nuclei wave functions

In many cases, the inclusion of anharmonic effects in the nuclei dynamics is crucial to properly describe the physics of solids. This happens, for example, when light atoms are present, like in organic semiconductors and perovskites (of technological interest for photovoltaic and thermoelectric applications) and in hydrides (among which we have the highest critical temperature superconductors discovered so far). The stochastic self-consistent harmonic approximation (SSCHA) is an efficient method to include this effects in ab initio calculations. However, a full exploitment of this method to provide anaharmonic corrections to the nuclei wave functions is still missing. This could be very useful to correctly estimate quantities of physical interests, like the zero-point and the temperature-dependent electron energy bands (gap) renormalization, and the phonon-mediated optical transitions. The aim of the project is to develop the theoretical structure and the numerical implementation of the SSCHA method to obtain the anharmonic corrections to the nuclei wave functions. The first task will be the implementation of the method for simple 1D models with generic anharmonic potentials, with the aim of comparing the exact wave function (obtained by solving numerically the Schrodinger equation) with the SSCHA anharmonic wave function computed with higher and higher order corrections. By the end of the project, the candidate will acquire knowledge in numerical methods and in phonon anharmonicity (and in particular in the SSCHA method).

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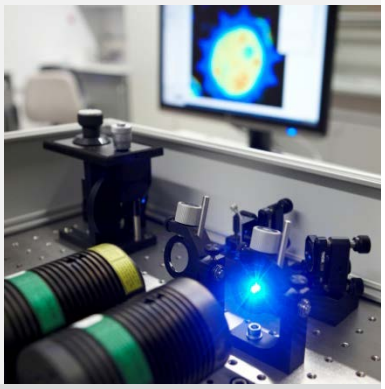
12 Anisotropic phonon polaritons in biaxial van der Waals materials



Low-dimensional van der Waals (vdW) materials have recently been attracting a substantial interest regarding photonics and optoelectronics applications since they support a variety of polaritons – oscillating dipolar excitations coupled to electromagnetic fields. Polaritons in vdW materials have different phase and group velocities in different directions, thus being strongly anisotropic. The project will study exciting exotic phenomena caused by the anisotropic polaritons, such as negative refraction, supefrocusing, slow light, etc.

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13 Theory of optical nanocavity-molecule interaction

Plasmons in nanocavities and nanoparticles are collective excitations of conduction electrons at the surface of metals that give rise to resonant surface charge density oscillations at optical frequencies. These excitations induce extreme localization and enhancement of optical near fields, beating the diffraction limit and thus enabling the field of nanooptics. When a molecule is located in the proximity of a plasmonic nanoparticle, the electronic and vibrational excitations of the molecule can be dramatically enhanced and modified. The theoretical description of this effect requires the development of tools that involve methods from classical electrodynamics (to describe the optical response of a nanosystem) , condensed matter physics (to describe the many-body properties of the plasmons), quantum chemistry (to describe the properties of molecules) and quantum nanooptics (to describe aspects of coherence of the plasmonic light). We plan to tackle some of these methodological aspects to improve our understanding of the nanocavity-molecule interaction.

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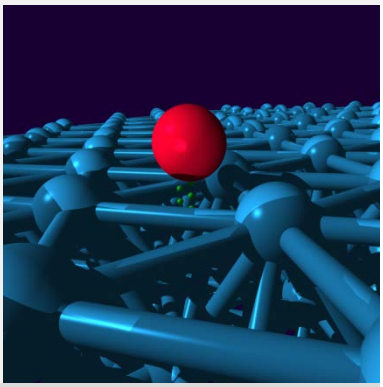
14 Ultrafast adsorbate vibrational dynamics



Ultrafast visible-infrared sum frequency generation (SFG) is a widespread technique that allows us to monitor the transient changes of adsorbates on surfaces. The recorded vibrational spectrum, characterized both by the frequency and the linewidth, brings information on the adsorption site, orientation of the adsorbed molecule, as well as on its interaction with the surrounding adsorbates and the surface. On metals, the lifetime of the vibrational excited adsorbates is strongly reduced due to the efficient excitation of electron-hole pairs. The aim of this master thesis project is to investigate from a theoretical point of view how this vibrational linewidth depends on various factors such as, the crystal face and surface coverage. The student will use two different approaches that are both based on density functional theory, namely, ab initio Langevin dynamics and density functional perturbation theory.

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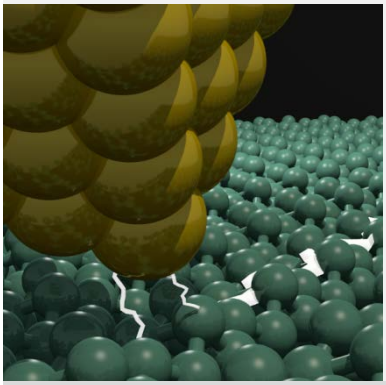
15 Quantum transport and spin physics in graphene nanostructures

Graphene nanostructures (GNS) show fascinating properties, including the possibility to develop intrinsic pi-paramagnetism from topological frustrations defined by their atomic structure. Nowadays synthetic chemistry and surface science techniques allow to produce and characterize such atomically precise GNS adsorbed on substrates. This situation makes GNS real and interesting candidates as elementary active components of a new generation of nanoscale quantum spintronic devices. In this theoretical project we will develop and apply computational approaches to predict properties of experimentally relevant compounds. A simple, yet highly successful, description of such systems is tight-binding and meanfield Hubbard models. We will compute topological properties and spin states of specific GNS and explore how they affect electron quantum transport through them, e.g., by injecting tunnelling currents from the tip of a scanning tunnelling microscope.



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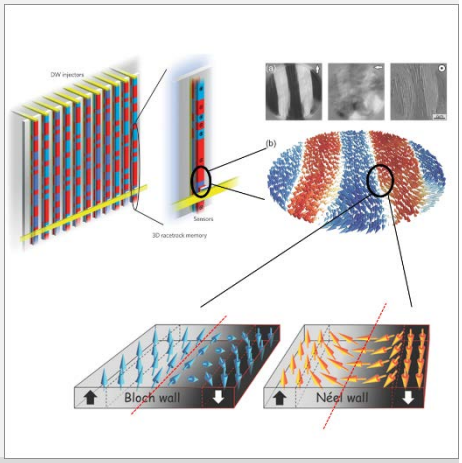
16 The Dzyaloshinskii-Moriya Interaction in ultrathin films



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The spin-orbit interaction is at the origin of the antisymmetric exchange interaction between spins known as the Dzyaloshinskii-Moriya Interaction (DMI). Since it favours canted orientations of neighbouring spins, the DMI can result in exotic spin structures in the nanoscale that show chirality, i.e. handedness, such as spin spirals and skyrmions. This property of chirality is the foundation for many spin-based technologies.

Inversion symmetry breaking is a necessary condition for DMI. Therefore, we often find it localized at surfaces and interfaces. In the case of a layered heterostructure, if the layers are thick enough, the interfacial DMI contributions are essentially two-dimensional and independent of each other. This is not the case in the limit of ultrathin layers, where perpendicular chiral interactions are not quenched. As a consequence, screw-like rotating spirals and lateral displacement of skyrmions are predicted. During this Master Thesis project, we will study the DMI in this ultrathin limit by means of ab initio calculations. Our goal is to determine the DMI at the atomistic level, i.e. to have access to the tensorial exchange coupling constants themselves, and to understand the DMI dependence on the electronic structure.

17 Hybrid perovskites for photovoltaics – stability and degradation mechanisms

Hybrid perovskites constitute a new class of energy materials whose photovoltaic response already exceeds 25%, *on par* with current (yet far more costly) silicon-based technologies. As such, these soft molecular solids offer the exciting prospect for the large-scale production of cheap, efficient, and flexible next-generation solar cells. Beyond their exceptional ability to harness the power of the Sun, they are also finding new applications in optoelectronics, quantum technologies, sensors, or memory devices. At present, the primary hurdle for their widespread use relates to their poor structural and chemical stability, also making the discovery of new candidates with improved performance a largely blind and labour-intensive endeavor. As part of wider research efforts using state-of-the-art experimental and computational techniques, the student will explore the physico-chemical mechanisms underpinning the stability and degradation of these materials under realistic conditions, with a view to attaining a detailed understanding of these processes at the atomic and molecular levels.

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18 Exploring the growth and the electronic structure of in-plane heterostructures of transition metal dichalcogenides

The objective of this Master project is to create a hybrid system of two transition metal dichalcogenides (TMDs) with different electronic affinity, e.g. MoSe2 and WSe2 on Au(111) surfaces and explore the union between them. The interesting aspect about these materials is that the boundaries between two of them can be very abrupt, and a p-n semiconductor junction can be created at the scale of a few atomic distances. The spectroscopic analysis of these systems with a low-temperature Scanning Tunneling Microscope (LT-STM) will be the fundamental element to demonstrate that a band shift occurs at the junction and to characterize the electric fields that can be generated in it. The student will optimize the growth of two different p-type and n-type TMDs semiconductors on a Au(111) surface by molecular beam epitaxy, characterize the resulting film morphology by atomic force microscopy and ultimately study TMDs heterojunction boundary electronic properties by LT-STM. All the different experimental techniques are at hand to the student in the CFM.

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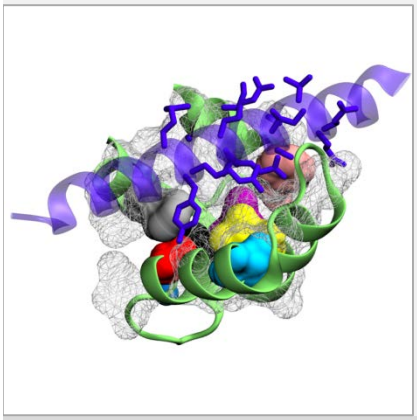
19 Molecular dynamics study of Calmodulin

The complete resolution of the sequence of the human genome in 2016 has been a huge milestone that continuously reveals causal relations among pathologies and gene signaling. Moreover, the latest advances of experimental techniques, such as nuclear magnetic resonance, provide a direct access to 3D maps with atomic resolution of the proteins that form cell membranes. This new accessible structural information has become a revolution in biological sciences for the design of new drugs that improve the well-being of humans. Remarkably, 60% of the commercial drugs act precisely on the proteins located at the cell membranes. With this scenario in mind, physical models that mimic atomic interactions within the proteins and their posterior time evolution through molecular dynamics provide a very powerful tool for the prediction and comprehension of membrane phenomena. Theoretical simulations of proteins serve as a guidance for the design of new drugs and help understanding the enormous amount of experimental information available. In this Master Thesis we shall consider the Kv7.2 channel of neuron membranes — a potassium voltage-gated channel located in human neurons —whose functioning relies in a potential difference induced by calmodulin (CaM). By means of All-atom simulations, molecular dynamics and coarse grain models, we would like to validate two claims regarding the behavior of the secondary structure of the IQ motiv of the channel: 1) Both wild type and mutant can form stable helices without the ribosome; 2) Wild type can form an alpha helix at the ribosome whereas the mutant cannot.



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