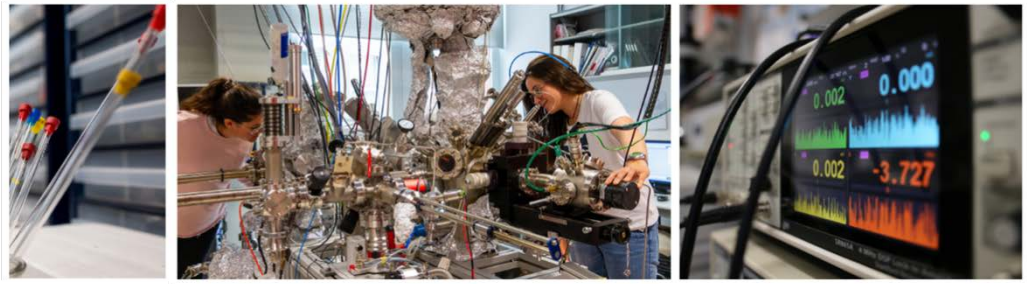

MASTER THESIS OFFER 2022/2023

1. **Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications**
2. **New Photoactivated Synthesis Routes to Single-Chain Nanoparticles**
3. **Theory of optical nanocavity-molecule interaction**
4. **Molecular mobility in simplified Industrial ternary mixtures for tire applications**
5. **Anisotropic phonon polaritons in biaxial van der Waals materials**
6. **Nanostructured materials for artificial photosynthesis**
7. **Quantum transport and spin physics in graphene nanostructures**
8. **Hybrid perovskites for photovoltaics – stability and degradation mechanisms**
9. **Anharmonic effects on the nuclei wave functions**
10. **Optical and thermal characterization of PIC plasmonic components**
11. **Molecular dynamics study of Calmodulin**
12. **Optical properties of 2D materials with ab-initio methods**
13. **Physical – chemical synthesis and characterization of hetero-interfaces of two dimensional materials**
14. **Cyclic polymers for biomedical applications**
15. **Electronic band structures of furan and thiophene nanothreads**

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 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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4 Molecular mobility in simplified Industrial ternary mixtures for tire applications

Blending polymers with other polymers or smaller molecules is an efficient tool to obtain new materials with tailored properties. Particularly, in the tire industry blending is used in connection with the fine-tuning of the glass-transition temperature to modify mechanical properties of materials. The final aim is to reduce the rolling resistance and increase the dissipation of energy during a braking period. These phenomena involve two distinct ranges in terms of frequency of deformations (around 100 Hz during rolling and around 1MHz on braking). Therefore, the understanding of the molecular dynamic behavior of the tire material in these frequency ranges is key to improve the mechanical properties of the rubber blend. In this project we like to explore whether the approach developed during last years for the understanding and modelling of the behavior of binary mixtures can be extended to the case of more realistic ternary mixtures. This project will be performed in collaboration with Michelin company and will involve differential scanning calorimetry and dielectric relaxation as two main experimental techniques.

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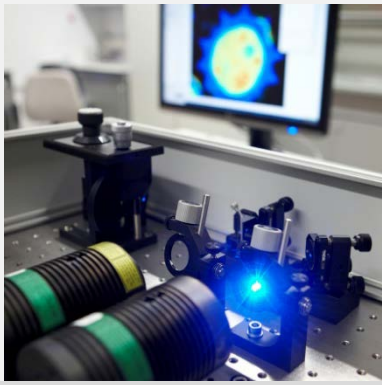
5 Anisotropic phonon polaritons in biaxial van der Waals materials



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 negativge refraction, supefrocusing, slow light, etc.

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6 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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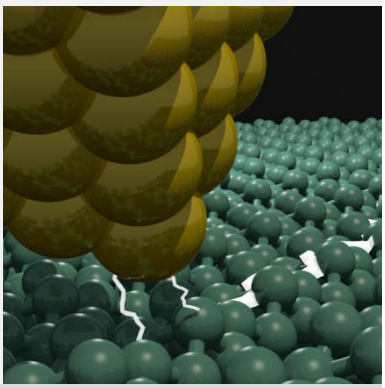
7 Quantum transport and spin physics in graphene nanostructures



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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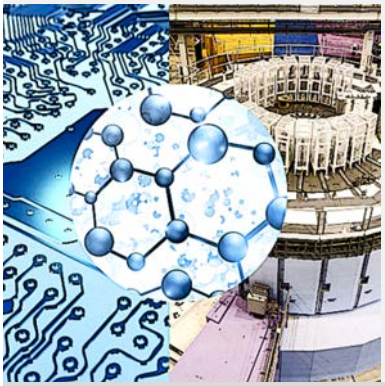
8 Hybrid perovskites for photovoltaics – stability and degradation mechanisms

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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9 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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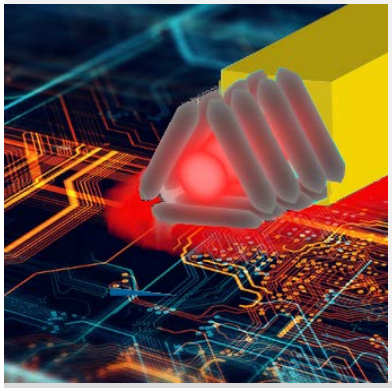
10 Optical and thermal characterization of PIC plasmonic components

Through the fast development and miniaturization of electronic devices, there has been an increased interest in studying Photonic Integrated Chips (PIC) in order to use them in new technologies, such as in quantum computing or in ultra-fast and ultra-secure communications. Plasmonic nano-devices, such as antennas and SPP (Surface Plasmon Polariton) waveguides, have been explored as promising components in PICs due to their high localization of electromagnetic energy and the overcoming of the diffraction limit of light in contrast with semiconductor integrated circuits, for instance. On the contrary, the use of plasmon components in reduced spaces could cause temperature rising as in the semiconductor chips. Therefore, thermal characterization of plasmonic components in chips is mandatory. The aim of this Master Thesis project is to perform a theoretical study of the optical properties and thermal dissipation of plasmonic nanoantennas and SPP waveguide configurations.



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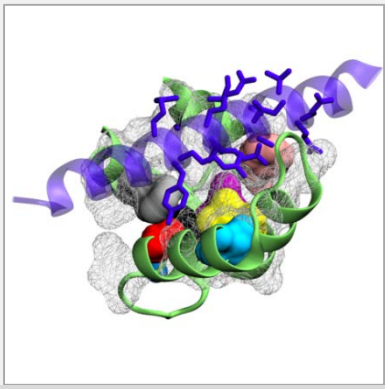
11 Molecular dynamics study of Calmodulin



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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.

12 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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13 Physical – chemical synthesis and characterization of hetero-interfaces of two dimensional materials

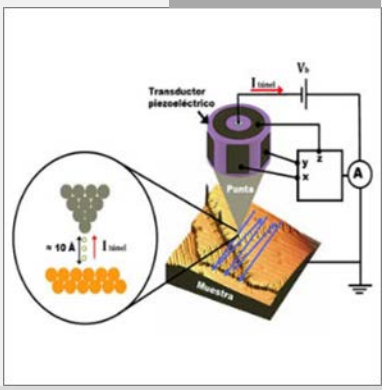
Two-dimensional materials are rising considerable attention in diverse fundamental and applied fields as energetics and photosensors, and charge transport, magnetism, and exotic superconductivity. The still young research field and the potentialities emerging at two-dimensional carbon-free materials demand for new tools and methods to control their electronic properties through interface engineering, chemical doping, control of defects, layer strain and compression of the structure, etc.

Subject of this master-thesis work is the formation and characterization of 2D-layers of metal halides, which show strong light absorption and sensitivity being fundamental elements for energy conversion and photodetectors. The material will be synthesized by vapor deposition in ultra-high vacuum. This protected environment enables a free choice of materials for the formation of heterostructurures (both organics and inorganics), control of their shape and size, doping etc. This is part of an on-going work focusing on the characterization of the structure (at atomic level), electronic and chemical properties occurring at these interfaces.

During this project, the student will be trained in various surface science techniques. She/he will acquire various skills, which include handling ultra-high vacuum equipment preparation of the sample preparation via physical vapor deposition, sample characterization via Auger spectroscopy and state of the art scanning probe techniques at cryogenic temperatures (liquid nitrogen and liquid helium).

+ INFO

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



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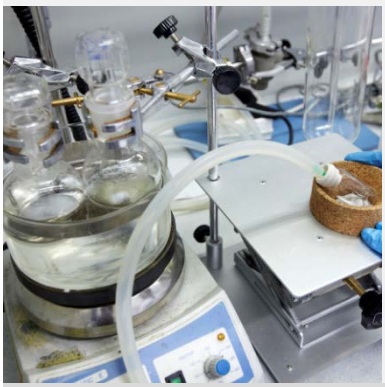
14 Cyclic polymers for biomedical applications

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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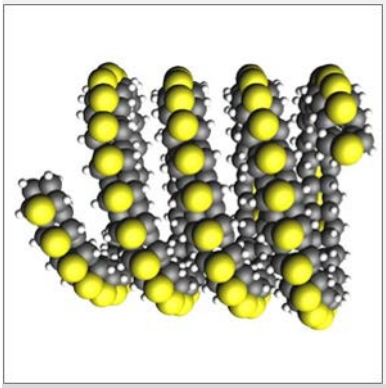
15 Electronic band structures of furan and thiophene nanothreads

Nanothreads are highly extended one-dimensional molecules with cage-like bonding, akin to the thinnest possible threads of diamond and capped by circumferential hydrogen. One of the defining features of nanothreads is the unique combination of extreme thinness (only a few Å in diameter) and rigidity (multiple covalent bonds connecting each unit). This feature distinguishes nanothreads from traditional polymers that are generally flexible and nanotubes that are much thicker. In 2014, Nanothreads were first made by high pressure-induced polymerization of benzene at 20GPa. Other small aromatic molecules such as pyridine, furan and thiophene also form nanothreads under similar conditions.

Following the [4+2] cycloaddition pathway in the synthesis, the structures of thiophene (or furan) threads may have the S (or O) atom residing all on the same side or on opposite sides (alternating every other, every pair, or more complex patterns) of the threads (see figure). The overlap between the pz orbitals on the S (or O) atom may give rise to interesting electronic properties. The student will work on using electronic structure code to optimize the geometries of these threads and calculate their band structures, and study the substituent effects on the geometry and electronic structures of these threads.



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