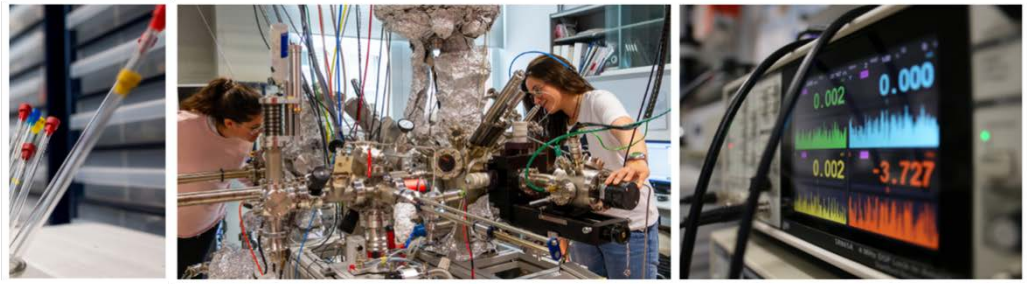

MASTER THESIS OFFER 2023/2024

1. **Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications**
2. **Design and synthesis of highly polar polymers (HPPs) for energy storage applications**
3. **Theory of optical nanocavity-molecule interaction**
4. **Optical properties of 2D materials with ab-initio methods**
5. **Anisotropic phonon polaritons in biaxial van der Waals materials**
6. **Emerging chip-scale quantum emitters for applications in quantum technology**
7. **Quantum transport and spin physics in graphene nanostructures**
8. **Hybrid perovskites for photovoltaics – stability and degradation mechanisms**
9. **Phonon Anharmonicity: From High-Temperature Superconductivity to Charge Density Wave Transitions and Thermal Conductivity Calculations**
10. **CO-O recombination at surfaces studied with machine learning potentials based on first-principles**
11. **Molecular dynamics study of Calmodulin**
12. **Interaction of intelligent drug delivery vehicles with model biomembranes**
13. **Physical – chemical synthesis and characterization of hetero-interfaces of two dimensional materials**
14. **Cyclic polymers for biomedical applications**
15. **Engineering of superconducting gap states**
16. **Electronic band structures of furan and thiophene nanothreads**
17. **Genetic algorithms for enhanced chiral sensing**
18. **Local probing of molecular mobility by means of a AFM-based technique**
19. **Optically-driven self-oscillating matter**
20. **Quantum Coherent Transport in Superconducting Nanostructures**

Updated on 31/03/2023

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 Design and synthesis of highly polar polymers (HPPs) for energy storage applications

In a world that is seeking alternative, eco-friendly energy sources, and reduced CO2 emissions, harvesting energy that is wasted in our environment becomes increasingly important. Efforts on electrical energy storage technologies are growing on par with those on energy generation from renewable sources due to the intermittent nature of their output. Currently, batteries and capacitors are the main types of devices used for electrical energy storage. Precisely, one important part of this project is to enhance the performance of ferroelectrics to fuel the ecological transition towards highly efficient electrical energy storage devices. Polar polymers have emerged as promising versatile materials for a wide variety of energy storage applications, allowing to obtain relatively high dielectric constants. Functional groups with high dipole moments (e.g., –F and –CN) tend to result in materials with increased dielectric constants.

The aim of this Master Thesis is the development of new ferroelectric Highly Polar Polymers (HPPs) to be used in capacitors. The proposed strategy relies on the design and preparation of new protonated/deuterated (h/d) cyanide-based polymers (linear precursors and Single Chain Nanoparticles) as potential ferroelectric materials for energy storage application.

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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 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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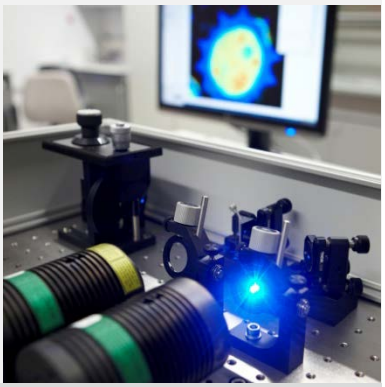
5 Anisotropic phonon polaritons in biaxial van der Waals materials



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 negative refraction, superfocusing, slow light, etc.

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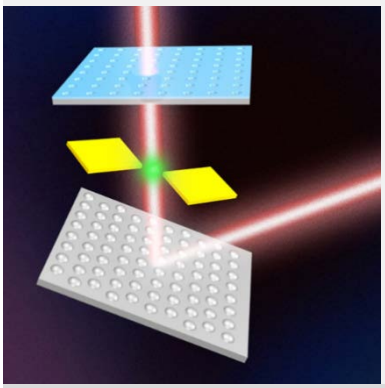
6 Emerging chip-scale quantum emitters for applications in quantum technology

Quantum technologies are one of the fastest growing scientific fields of the last decade, including quantum information, quantum computing and communication. This growing field requires the use of non-classical light sources, i.e., sources that produce photons with controlled quantum correlations. These non-classical light generators are based on quantum emitters, a sources of correlated single photons or pairs of entangled photons. One of the most promising platforms for the fabrication of such emitters are semiconductor quantum dots, which combine inherent quantum optical properties with the versatility and scalability of a solid-state material. Particularly, quantum emitters based on hybrid quasi-particles, combining of plasmons and excitons, present a very promising approach to overcome the existing limitations of the state-of-the-art nanostructured systems. These hybrid emitters can be developed using quantum dots and metallic nanostructures operating in the light-matter interaction mode as efficient light-driven sources of single and entangled photons.

The main goal of the present project is to design and implement highly efficient hybrid plasmon-exciton quantum emitters operating as on-demand sources of pure single indistinguishable photons and/or pairs of entangled photons. The project is essentially experimental, but can be combined with theoretical modelling. This includes the combination of nanomaterial preparation and processing techniques, optical spectroscopy at the single quantum dot level and single photons manipulation. In addition to gaining new knowledge and experience, the project offers a unique opportunity to conduct mid-scale but important research in the field of quantum technologies.



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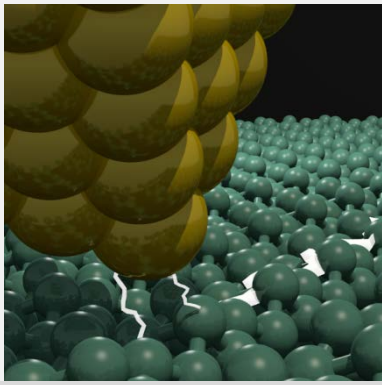
7 Quantum transport and spin physics in graphene nanostructures



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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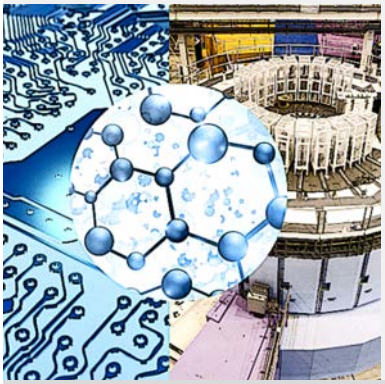
8 Hybrid perovskites for photovoltaics – stability and degradation mechanisms

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 Phonon Anharmonicity: From High-Temperature Superconductivity to Charge Density Wave

In this master project the student will learn to calculate from first principles methods structural, thermodynamic, spectral, transport, and/or superconducting properties of materials in systems where lattice vibrations are strongly anharmonic. In fact, strong anharmonicity is present in high-temperature superconducting hydrogen-based compounds, materials undergoing a charge density wave (CDW) or ferroelectric transitions, thermoelectric materials, and so on. The student will have the option to work on different topics, such as i) the prediction or characterization of new hydrogen-based superconductors; ii) the characterization of CDW transitions in materials relevant for topological electronic properties, both in the bulk or in the 2D limit; iii) the calculation of thermoelectric properties of materials in the bulk or in the monolayer; or iv) the analysis of the mechanical properties of 2D membranes like graphene, which still remain largely controversial.

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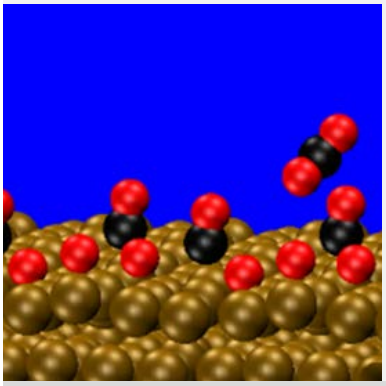
10 CO-O recombination at surfaces studied with machine learning potentials based on first-principles

Recombination processes involving gas-phase and pre-adsorbed species on surfaces play a prominent role in a huge variety of natural and technological processes: in the production of chemical compounds, in the search for controlling the emission of noxious gases, and in the research on hydrogen storage, to just cite some relevant examples in which they are exploited from the catalysis perspective. In this project, we propose to investigate the recombination of O with preadsorbed CO. There are experiments showing that the efficiency of these process depend dramatically on the metal surface considered and on coverage. The objective will be to determine the origin of such dependence by constructing machine learning potentials of the O+CO-surface interaction, in which to perform high dimensional molecular dynamics simulations for several coverages and surfaces of interest. The student will learn about theoretical chemical physics, including density functional theory, electronic structure calculations, molecular dynamics methods, scientific programming, and machine learning techniques.



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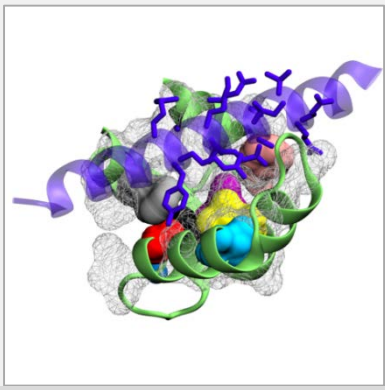
11 Molecular dynamics study of Calmodulin



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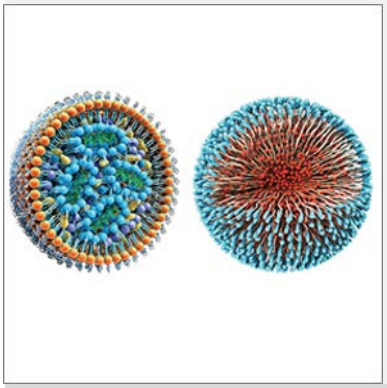
The complete resolution of the sequence of the human genome in 2016 has been a huge milestone that continuously reveals causal relations among pathologies and gene signaling. Moreover, the latest advances of experimental techniques, such as nuclear magnetic resonance, provide a direct access to 3D maps 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 Interaction of intelligent drug delivery vehicles with model biomembranes

Many of the therapies or modalities emerging from pharmaceutical companies, including precision cell-based therapies, rely on being delivered directly into the cytosol or alternatively to specific sub-cellular compartments within the cell, for their activity. Unfortunately, however, many of the modalities are impermeable to the cell membrane. Despite the considerable research effort that has gone into the development of intelligent delivery systems, the field is currently hindered by a poor understanding of how the vehicles gain access to the interior of the cell. In this Master thesis project, responsive nanoparticulate delivery systems composed of lipid and polymeric nanoparticles will be assembled and characterized. Their interaction with in vitro biomimetic cell membranes of different complexity will be also studied by a combination of imaging (confocal and atomic force microscopy) and scattering methods.



Contact: **Armando Maestro**
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13 Physical – chemical synthesis and characterization of hetero-interfaces of two dimensional materials

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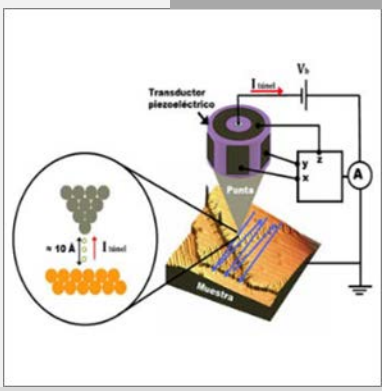

Two-dimensional materials are rising considerable attention in diverse fundamental and applied fields as energetics and photosensors, and charge transport, magnetism, and exotic superconductivity. The still young research field and the potentialities emerging at two-dimensional carbon-free materials 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).

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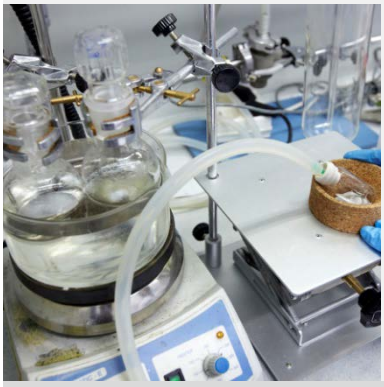
14 Cyclic polymers for biomedical applications

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 Engineering of superconducting gap states

The subject of this master's work is the study of in-gap states in superconductors when mangetic impurities are present on its surfaces. This is part of the on-going experimental and theoretical effort of the group Quantum Phenomena on Surfaces at CFM-MPC. The aim of the study is to be able to generate electronic structure with increasing complexity as magnetic impurities are manipulated with a scanning tunneling microscope to create magnetic nanostructures. This strategy is what recently has benne term as reserach on "Designer Quantum States". The idea is to be able to create new states of matter that have special properties by marrying topology and quantum entanglement. This is particularly easy on superconductor susbtrates because their gound state is already a complex many-body entangled state. The object of the master is two-fold. First work with Bogolioubov-de Gennes equations to compute intricate in-gap electronic structure. Second porpose experiments that can be performed in an STM setup.

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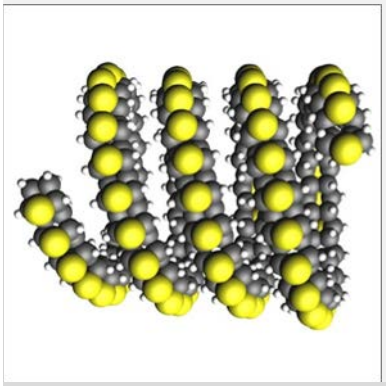
16 Electronic band structures of furan and thiophene nanothreads

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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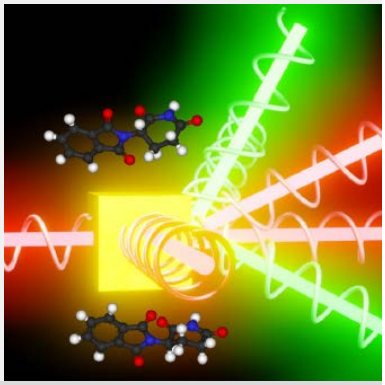
17 Genetic algorithms for enhanced chiral sensing



Contact: **Jorge Olmos Trigo**
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In this project, the student will become familiar with the Physics of chiral sensing. Chirality is a geometrical property in which an object is not superimposable with its mirror image. In the Pharmaceutical industry, chiral specificity is critical because opposite enantiomers, i.e., mirror pairs of chiral molecules, can have beneficial or detrimental biological effects on our body. Although they share the same atomic composition, enantiomer pairs are indistinguishable when measuring their scalar physical properties. Their chiral nature is revealed mainly by interacting with another chiral entity. In electromagnetism, the most common chiral entity is the helicity, the handedness of the wave. Metasurfaces, i.e., flat arrays of antennas designed to control the properties of light, are promising candidates for revealing and enhancing the spectroscopic signals of enantiomers. The underlying phenomenon is that metasurfaces can be designed to enhance the electromagnetic fields associated with a given optical helicity. However, which is the best antenna to enhance electromagnetic fields with the desired optical helicity?

In this project, the student will answer this question both analytically and numerically. In particular, the student will use (quantum) genetic algorithms, a numerical method for solving constrained optimisation problems based on natural selection, to get insight into the best candidate for enhanced chiral sensing. In addition, the student will be in close contact with the Quantum Nanophotonics Laboratory, led by Gabriel Molina-Terriza, to eventually corroborate his/her findings with feasible experiments. Last but not least, this project aims to be a scientific paper that will see the light of day at the end of the project.

18 Local probing of molecular mobility by means of a AFM-based technique

Polymers and soft matter in general are characterized by significant molecular mobility, which can be probed by a variety of experimental techniques. However, in many materials the molecular mobility is highly heterogeneous and conventional approaches fail to provide site-resolved information. In this project, an AFM-based experimental approach developed during the last years will be applied to characterize the molecular mobility in nanostructured polymeric materials.

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19 Optically-driven self-oscillating matter

Self-oscillations are periodic changes of a system state under a non-periodic stimulus. Although self-oscillation is the fundamental features in many biological systems (e.g., neuron firing, heart beating) it remains poorly explored in synthetic materials. The increasing attention of the community to the design and experimental development of self-oscillating matter is motivated by the potential use of such systems in emerging technologies (e.g., light engines, self-actuators, sensors). The aim of this project is the rational design and development of a hybrid colloidal particles comprising thermoplasmonic components (plasmonic nanocrystals) and thermoresponsive host matrix (agarose) to study the emergence of light-sustained self-oscillatory signatures down to single colloid level. The project is multi-disciplinary and involves a variety of techniques: fabrication of nanostructures, optical characterization, and the use of advanced optical techniques such as optical trapping. The student will receive a comprehensive training in experimental nanochemistry, optical microscopy techniques, and data science.

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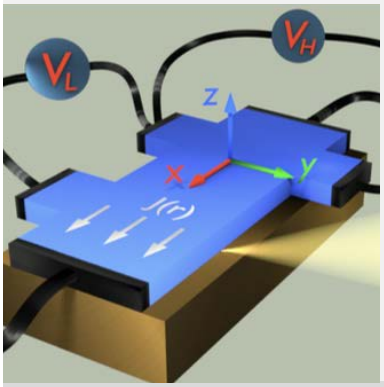
20 Quantum Coherent Transport in Superconducting Nanostructures

In this project, the successful candidate will have the opportunity to develop an effective model for studying transport properties in hybrid superconducting and metallic structures. This research aims to support experimental activities at the Center for Materials Physics and Nanogune, specifically on low-dimensional Josephson junctions, and will allow for exploration of cutting-edge topics in the field of quantum transport in nanostructures. During the project, the candidate will focus on coherence and electronic interference effects in multiterminal structures, which are essential for understanding the behavior of these systems. They will begin by mastering theoretical tools such as the scattering matrix and semiclassical transport equations. With these tools, they will be able to calculate charge, spin, and heat currents as functions of external parameters, such as voltage, magnetic field, and temperature. The successful candidate is expected to have basic knowledge in Quantum Mechanics and Condensed Matter Physics. The work will be carried out in collaboration with the researchers of the Mesoscopic Physics Group, who will guide the candidate through the project and provide support and insights into its main goals.



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