MPC/DIPC Scholarships for Master in Nanoscience 2020-2021

MPC/DIPC offers Scholarships to accepted students in the Master in Nanoscience.

These are the conditions:

1) **Deadline** for Application: 30th June 2020

2) **Amount**: 3.000 euros

3) **Requirements**:

(i) Having been accepted in the Master in Nanoscience program 2020-2021

(ii) Having confirmed by email the acceptance

(iii) Acquire the compromise to choose a Master Thesis project in any of the CFM, UPV/EHU or DIPC research groups offer. The offer will be updated from this year offer shown at the end of this document.

4) **Documents**: updated CV including both academic and research records, personal and contact data.

5) **Resolution date**: 30th July 2020

Applicants should send the documents by email to

andres.arnau@ehu.eus or info@mscnano.eu

CFM, UPV/EHU and DIPC MASTER THESIS OFFER 2019-2020

(1) **Title**: Electron and phonon transport in multi-terminal graphene-based devices

Description: The physics of nanoscale electronic devices is interesting from both fundamental and applied perspectives. In this project we study quantum transport theory based on nonequilibrium Green's functions and apply it to compute electronic and phononic conductivities in multi-terminal setups, i.e., nanoscale junctions connected to two or more electrodes. Focus will be on 2D graphene-based structures and networks, e.g. perforated graphene or interconnected graphene nanoribbons, with the goal to understand and engineer their basic electronic and phononic properties.

Contact: Thomas Frederiksen (DIPC)

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(2) **Title**: Physics and Chemistry of Curved Crystal Surfaces: oxygen, carbon monoxide and carbon dioxide chemisorption and dissociation on stepped surfaces.

Description: 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 CO2 we the role of active step sites during gas-metal interactions for the most relevant catalytic processes, namely CO oxidation and CO2 dissociation. 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.

Contact: Enrique Ortega

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(3) **Title**: Effects of electron-electron interaction by stacking two-dimensional materials

Description: 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 role of electron-electron interaction when having several layers of graphene either independently or sandwiched with other two-dimensional materials.

Contact: Andrés Ayuela

Email: swxayfea@sw.ehu.es

(4) **TITLE**: Charge-Density-Wave Transitions in Topological Materials from First Principles

BRIEF DESCRIPTION: The goal of this project is to discover new topological materials, whose non-trivial topology can be controlled with temperature or strain. Such type of materials can provide a way of engineering devices where the robust properties of topological materials can be switched on/off. We will make use of first-principles calculations to seek for materials with non-trivial topologythat undergo a charge-density-wave (CDW) transition. A CDW is a structural phase transition that can modify the electronic properties. Since CDWs can be controlled with temperature and/or strain, materials undergoing CDW transitions are perfect candidates.The phase diagram of candidate materials will be determined explicitly calculating the CDW transition temperature with the stochastic self-consistent harmonic approximation, which rigorously includes quantum and anharmonic effects, crucial in CDWs. We will also study the symmetry of the system and band topology of electronic states, as well as the gap functions when the CDW occurs.The candidate will acquire a deep knowledge in advanced group theory, modern theory of topological materials, and phonon anharmonicity.

CONTACT PERSON: Ion Errea and Maia G. Vergniory

CONTACT EMAIL: ion.errea@ehu.eus and maia.garcia@ehu.eus

(5) TITLE: Anisotropic phonon polaritons in biaxial vad der Waals materials

BRIEF DESCRIPTION: 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.

CONTACT PERSON: Alexey Nikitin

CONTACT EMAIL: alexey@dipc.org

(6) **Title**: Cyclic polyethers for decorating metals surfaces

Description: Cyclic polymers possess unique physico-chemical properties compared to their linear counterparts as a result of the absence of end-groups. These differences may be expressed in their hydrodynamic, rheological, optical and thermal properties. _ENREF_1The student will synthesize cyclic polyethers and polymer-decorated metal surfaces by using a combination of techniques including those needed to generate cyclic polymers containing thiol groups via ring closure approaches as well as those needed to generate polymer-decorated gold surfaces. The student will learn state-of-the art techniques for characterizing polymers with complex structures (MALDI-TOF MS, GPC with triple detection, NMR, FTIR and Raman spectroscopy) and for characterizing metal surfaces and metal colloidal particles (XPS, UV-ViS and contact angle).

Contact: Fabienne Barroso-Bujans

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(7) **Title**: Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications

Description: 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.

Contact: José A. Pomposo

Email: josetxo.pomposo@ehu.eus

(8) **Title**: New Photoactivated Synthesis Routes to Single-Chain Nanoparticles

Description: 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.

Contact: José A. Pomposo

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(9) **TITLE**: Nanostructured materials for artificial photosynthesis

BRIEF DESCRIPTION: 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.

CONTACT PERSON: Yury Rakovich

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(10) **Title**: Nanoelectrical properties of polymer electrolytes

Description: Solid polymer electrolytes are the key to develop efficient new generation batteries. The electrolyte must comprise a series of important requisites. They should not only provide suitable charge transport over a wide range of temperatures but also must maintain good chemical stability and compatibility with the electrode materials. In this work, the aim is to study the nanoelectrical properties of polymer electrolytes using Atomic Force Microscopy (AFM) based techniques. The AFM allows providing structural and electrical properties simultaneously, with a lateral resolution better than 40 nm. The AFM study will be complemented by macroscopic experiments. In this way, it will able to find possible links between the molecular response at the nanoscale, with the overall material properties in the macroscale.

Contact: Daniel Martinez-Tong and Angel Alegria

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(11) **TITLE**: Optical properties of 2D materials with ab-initio methods

BRIEF DESCRIPTION: 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.

CONTACT PERSON: Roberto D'Agosta

CONTACT EMAIL: roberto.dagosta@ehu.es

(12) **Title:** Engineering the reactivity of nanoporous graphene (NPG)

Description: Recently, a new multifunctional material has been reported [*Science 360. 199 (2018)*], which is composed of a graphene membrane with pores whose size, shape and density can be tuned with atomic precision at the nanoscale. In this work, state-of-the-art simulation tools will be used to investigate the modulation of the electronic properties of NPG by doping the pores with different heteroatoms. Special focus will be given to the enhancement of its chemical reactivity, which might be very useful for different applications, such as energy storage or catalysis. Besides, a strong collaboration with experimental groups experts in the field is envisioned.

Contact: Aran Garcia-Lekue

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(13) **Title**: Dimerized diamond chain in magnetic fields

Description: In this project, we will investigate the property of a dimerised diamond chain [1] closed in a loop geometry. We will examine the effect of an Aharonov-Bohm and transverse magnetic fluxes . Additionally, we will account for 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].

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).

Contact: Dario Bercioux (Mesoscopic Physics group)

Email: dario.bercioux@dipc.org

(14) **Title**: Ab initio calculation of molecules in a plasmonic cavity

Description: Using state-of-the-art first-principles methods based on time-dependent density functional theory (TDDFT), the student will study the properties of molecules in the proximity of metal nanoparticles and inside plasmonic gaps created by two neighboring nanoparticles. Special attention will be devoted to the influence of the presence of the molecule in the conductive properties of the gap between the nanoparticles, and how this modifies and couples to the plasmonic response of the system. Alternatively, we will explore the possibility to efficiently simulate surface enhanced Raman spectroscopy (SERS) using first-principles simulations.

Contact: Daniel Sánchez Portal

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(15) **Title:** Seeking 2D ferromagnets among transition metal dichalcogenides

Description: Among the large variety of properties of the newly discovered two-dimensional (2D) materials, magnetism has been only recently added to them (2017) with the isolation of CrI_3 and $CrGeTe_3$ down to the mono- and bilayer limit, respectively [1,2]. 2D magnets will be crucial for future engineering of artificial materials with tailored functionalities. Unfortunately, the few 2D magnets discovered so far lack of chemical stability when exposed to air as well as large Curie temperatures, which preclude their ultimate integration in spin-based devices. Therefore, the identification of stable (usable) 2D magnets is currently one of the most exciting cutting-edge fields of research in condensed matter physics and materials science.

In this project, we aim at finding 2D magnets among the transition metal dichalcogenides (TMD), a largely unexplored family of layered materials in this regard despite the exciting theoretical predictions of magnetic solutions for some of them in the single-layer limit [3]. The project offers the opportunity to grow several TMD candidates ($PtSe_2$, $CrSe_2$, etc) and carry out their electronic and magnetic characterization down to the atomic level. In particular, single layers of different TMDs will be grown by molecular beam epitaxy (MBE) on graphene-based substrates. The atomic-scale investigation of the electronic and magnetic properties of the MBE-grown 2D TMD materials will be mostly carried out by means of high-resolution scanning tunneling microscopy and spectroscopy (STM/STS) at ultra-low temperature (300 mK) and high magnetic fields (11T).

[1] Gong, *et al*., Nature 546, 265 (2017).
[2] Huang, *et al*., Nature 546, 270 (2017).
[3] Mounet, *et al*., Nature Nanotechnology 13, 246 (2018).

Contact: Marco Gobbi and Miguel M. Ugeda
Email: mmugeda@dipc.org (www.2dspm.com)

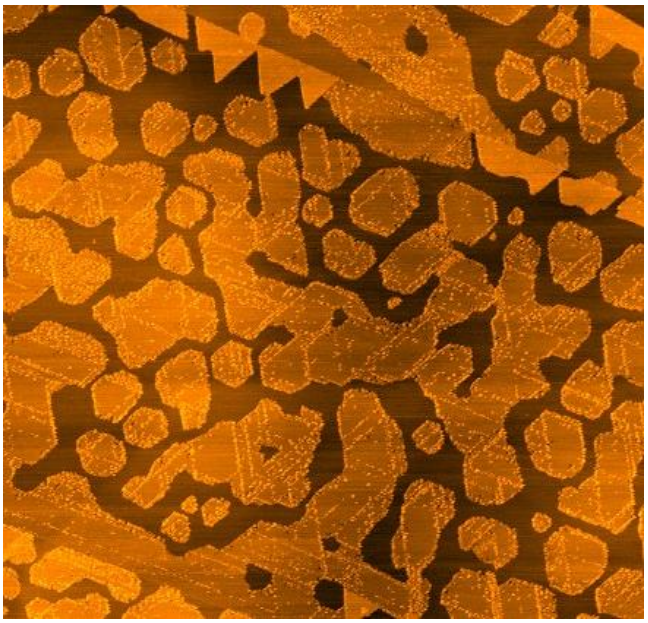

Figure.- AFM image of single-layer VSe_2 grown (MBE) in our lab. Size: 400 nm x 400 nm.

(16) **Title:** Impact of disorder in truly 2D superconductors

Description: Collective electronic phases are strongly dependent on the dimensionality of the system. For example, superconductivity survives in two dimensions (2D) due to the formation of vortex-antivortex pairs at low temperatures (Berezinskii–Kosterlitz–Thouless transition), a mechanism not present in conventional 3D superconductors. While the theoretical framework of 2D superconductivity was established several decades ago, its experimental realization in the ultimate 2D limit has only become possible since the recent advent of 2D materials.

Disorder - atomic defects in the crystal lattice - is intrinsically present in any material (…*nothing is perfect but real*). However, their impact on the most fundamental properties of a material becomes dramatic in low dimensions. This project proposes the atomic-scale investigation of the influence of disorder in single-layer $NbSe_2$, a recently discovered 2D superconductor [1]. The first part of the projects comprises the growth of single layers of $X_\delta Nb_{1-\delta}Se_2$ with minute amounts ($0 < \delta << 1$) of selected atomic impurities (X = Ir, Na) by molecular beam epitaxy (MBE). The degree of disorder in the 2D superconductor will be controlled by tailoring the δ parameter during the growth. In the second part of the project, the disordered 2D superconductors will be studied with atomic precision by scanning tunneling microscopy and spectroscopy (STM/STS) at ultra-low temperature (300 mK). We will map the fluctuations of the superconducting order parameter and phase in real space with atomic resolution. Furthermore, we will also explore the evolution of the superconducting and charge density wave states with disorder near the Anderson transition to the insulator state.

[1] Ugeda, *et al.*, Nature Physics 12, 92 (2016).

Contact: Miguel M. Ugeda
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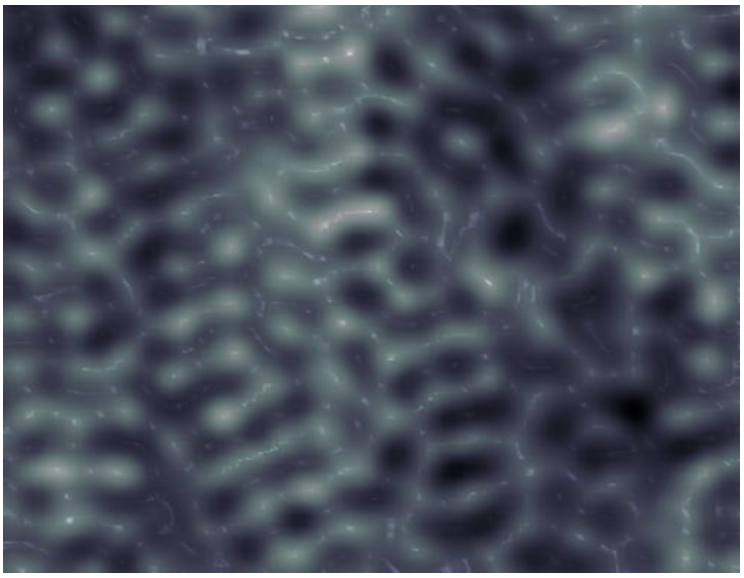

Figure.- Spatially resolved map of the fluctuations of the superconducting order parameter in single-layer $NbSe_2$ due to intrinsic disorder in the crystal lattice. The fluctuations show a wavelength of 0.7 nm. Parameters: 14 nm x 12 nm, T = 1 K.

(17) **Title**: Theory of plasmon-enhanced vibrational spectroscopy

Description: Plasmons are collective excitations of conduction electrons in metals that give rise to surface charge density oscillations at the metal-dielectric interface. Localized surface plasmons in metallic nanoparticles act as effective optical antennas that localize and enhance optical fields in subwavelength dimensions. When a molecule is located in the proximity of a plasmonic nanoantenna, its vibrational signal can be dramatically enhanced and modified. The theoretical description of this effect requires the development of theoretical tools that involve tools from condensed matter physics (to describe the properties of the plasmons), quantum chemistry (to describe the properties of molecules) and quantum nanooptics (to describe aspects of coherence of the plasmon-molecule interaction). We plan to tackle some of these methodological aspects to improve our understanding of experimental situations in plasmonenhnaced
molecular spectroscopy.

Contact: Rubén Esteban and Javier Aizpurua

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(18) **Title:** Ultrafast adsorbate vibrational dynamics

Description: 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.

Contact: Maite Alducin

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(19) **Title**: Theory of quantum sensing via spin Hall magnetoresistance in Pt thin films coupled to an array of spin qubits

Description: Mankind walks into the era of quantum technologies, where quantum devices extend the functionality of ordinary devices by utilizing our ability to prepare and control coherently quantum superpositions of states. Qubits are nowadays one of the most prominent examples of successfully implemented quantum devices, which exist in the labs of most world leading institutions and are awaiting for their practical use, not only for limited-scale quantum computing, but also for applications of a different and sometimes rather original nature, such as quantum sensing. In this project, we will consider the use of an array of qubits coupled to the environment as a means of constructing a highly sensitive spectral analyzer. The read-out signal is a simple resistivity measurement of a Hall-bar platinum device, which features a relatively strong spin Hall effect. Such spin-Hall-bar devices are routinely produced and measured in the group of Felix Casanova at CIC nanoGUNE and this project may stimulate interesting experiments in Donostia and worldwide. The project requires the student to become familiar with the ideas of quantum computing at a basic level (notion of qubit, state preparation, quantum gates, read out) and to use the available spin-Hall magnetoresistance theory to study how quantum sensing with qubits can be exploited for the benefit of constructing a spectral analyzer, which is capable of exploiting quantum superpositions to attain a sensitivity at or close to the quantum limit.

Contact: Vitaly Golovach

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(20) **Title**: New generation of memory and logic devices.

Description:
Non volatile memories on the track (race track memories) with chiral spin textures (skymions, domain walls and spin waves) as storage bits, can be manipulated by spin currents (via spin transfer and spin hall effect SHE). The aim of this master project is to investigate ultrathin magnetic multilayers, to fabricate and perform transport characterization of domain wall and spin wave dynamics in nanodevices.

References
(1) O. Gladii et al. , Spin Hall induced spin wave amplification in Py/Pt bilayers Appl. Phys. Lett. 108, 202407 (2016).

(2) D. Maccariello et al. , Electrical Signature of individual magnetic skyrmions in multilayered systems. Nature Nanotechnology, Nat. Nano 13, 233-237 (2018).

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