



Centro de Física de Materiales - CFM is a joint centre by the University of the Basque Country - UPV/EHU and the Spanish Research Council - CSIC. The centre brings together several outstanding teams who develop frontier research using state-of-the-art facilities.

CFM's headquarters is located at Ibaeta Campus in San Sebastian, within walking distance from several institutions also committed to explore physics and material science, both at fundamental and applied levels. Altogether, we represent a thrilling international community devoted to innovation and discovery at the very edge of science.

PhD Studentships

At CFM we are committed to provide future generations with the best opportunities to join the research community and develop high profile careers.

This is a unique occasion to work in an intellectually stimulating environment in close interaction with all our scientific staff, a large group of postdoctoral researchers and a wide network of international, world-class visitors.

We are currently seeking for bright, highly motivated students who will be able to make the best out of this opportunity. Candidates must show problem solving skills, as well as will to find and develop original and innovative solutions in unexplored domains of physics and material science. They are expected to integrate and contribute to all phases of scientific activity, from pure research to communication in international journals and conferences.

Next Deadline for Submission of Candidatures: 15th September 2014

Call is open for allocating 3 PhD studentships. Each studentship will cover a period of three years, including a salary of 15 972 € (before taxes) during the first year, with subsequent smooth increases over the next two. The studentship will also include a budget (allocated to the research group) covering research and training expenses. Studentships are funded by the Research Association MPC - Materials Physics Center.

PhD studentship will only be granted to successful candidates whose PhD project will be formally registered at the University of the Basque Country UPV/EHU before December 31st 2014 for the PhD contract to be continued.

Details about the available topics are provided in the following pages, together with general information on the application and evaluation processes.

<http://cfm.ehu.es/>

PhD Studentship Application Process

Interested candidates must send a CV, including an academic transcript with the marks obtained in the degree, and a brief statement of motivation.

Reference letters are welcome but not essential.

Please provide clear contact information and specify which is the research topic or topics you are applying for.

All documents must be sent to mpc@ehu.es

PhD Studentship Evaluation Process

Applications will be evaluated by a Committee designed by the CFM Direction Board. The following criteria will be applied (scoring weights are indicated in parentheses):

- CV of the candidate (65%)
- Adequacy of the candidate's technical background to the research line to which he/she is applying for (25%)
- Reference letters (5%)
- Diversity in gender (5%)

Only applications received before the deadline (15th September at 17:00 CEST) will be evaluated. Evaluation results will be communicated to the candidates soon after.

Positions will only be filled if qualified candidates are found. If this is not the case, the deadline for submission of applications may be extended.

Available Topics for PhD

• **The list of available topics is shown in the following pages.** Only three positions will be selected among all applications to any of these topics.

• You can apply for several topics simultaneously.

• When applying, please quote the reference(s) number (s) of the topic you are interested in.

• If you have specific questions, or need further information on an specific topic, please get in touch directly with the contact person mentioned in each topic description.

• For any general queries on the selection process, contact mpc@ehu.es.

Reference: PhD/2014/1

Electronic and magnetic properties of metal-organic coordination networks.

Contact person: Andres Arnau (andres.arnau@ehu.es)

The project will focus on the systematic theoretical study of structural, electronic and magnetic properties of different type of metal-organic coordination networks formed by 3d, 4d and 5d transition metal atoms and organic molecules with different shape, coordination and stoichiometry. Both first-principles DFT calculations and model hamiltonians will be used to describe the systems under study. Comparison with STS, ARPES and XMCD experimental data, when available, will permit to contrast the results of the calculations. It is recommended that the potential candidates have a basic knowledge of quantum mechanics, solid state physics and many-body theory, as well as fortran programming and computational skills using DFT codes, like VASP or SIESTA.

Reference: PhD/2014/2

Innovative routes to water-soluble bioactive single-chain polymer nanoparticles

Contact person: José A. Pomposo (Josetxo.pomposo@ehu.es)

The PhD student's research will be focused on the construction and characterization of water-soluble biofunctional single-chain polymer nanoparticles (SCNPs) by starting with well-defined polymer precursors synthesized by modern controlled radical polymerization techniques (RAFT polymerization) and by employing innovative intrachain folding/collapse methods to tune the compaction of the SCNPs towards globular bioactive enzyme-mimetic nano-objects. The candidate will have the unique opportunity to carry out his/her PhD Thesis at the frontier between chemistry, physics and biology in the "Polymers & Soft Matter" Group - PSMG.

Reference: PhD/2014/3

Chemical reactions on surfaces

Contact person: Celia Rogero (celia_rogero@ehu.es)

The project will focus in seeking new routes for the design and synthesis of molecular nanostructures, exploiting the catalytic activity which takes place at the surface of some materials. The outcome will provide fundamental understanding and concepts which can serve as basis for the development of several applications, such as heterojunctions, molecular superconductors and molecular magnets, efficient photovoltaic cells, etc. Through exploring, understanding and designing of new strategies for molecular growth, the project will contribute to consolidate several molecular technologies. The experimental activity linked to the project will consist in the combined use of a wide range of surface science techniques, such as XPS, STM, NEXAFS, UPS and AFM. Intense exchange and collaboration with several groups specialized in chemistry, chemical engineering and theoretical physics will take place during the project.

Reference: PhD/2014/4

Study of Structural Defects in Carbon-Based Nanostructures.

Contact person: Sebastian Bergeret (sebastian_bergeret@ehu.es) and Dario Bercioux (dario.bercioux@gmail.com)

The study of defects in carbon-based nanomaterials is important for a full understanding of the functionality of future devices based on these materials. For example defects in carbon nanotubes can confine electrons to quantum dots with an energy level spacing exceeding thermal broadening at room temperature.

In the framework of this project we are interested in investigating theoretically several properties related to the presence of defects and inhomogeneities in carbon based materials and their observation with STM/STS probes.

Specifically we plan several work packages, including:

- (a) Characterisation of the scattering states due to the presence of topological defects;
- (b) Effect of ad-atoms and adsorbates;
- (c) Electronic transport properties of defected carbon nano-structures;
- (d) Characterisation of phonons and electron-phonon coupling and their effects on quantum transport.

The project has a full duration of 3 years is designed in order to have a significant overlap with the research activities present at the CFM/MPC and other centers in Donostia.

Reference: PhD/2014/5

Interplay between structural and electronic properties of ultra-thin nanostructured films grown onto metallic substrates.

Contact person: Jorge Lobo Checa (jorge.loba@csic.es)

The offered PhD project involves basic experimental research in the field of Condensed Matter Surface Science. The focus of his/her investigation will be to unravel the fundamental properties of electrons in 1D or 2D superlattices at the nanometer range. To that end, the candidate will study in detail different nanostructured systems and correlate the exquisite balance between the existing structural morphology and its electronic bands. The proposed systems involve ultra-thin molecular and metallic films grown in-situ onto both:

- i) surface alloys, such as BiAg₂ or SnGe₂, and
- ii) curved crystals, characterized by a smooth variation of the local size of its terraces.

To carry out this research, the candidate must learn how to use a wealth of experimental techniques, with particular attention to Angle Resolved Photoemission Spectroscopy (ARPES), Scanning Tunneling Microscopy (STM), and Low Energy Electron Diffraction (LEED). All these techniques are based on ultra-high-vacuum (UHV) conditions. Part of this research will take place away from the home Institution and the candidate must be willing to travel outside for short stays at large scientific infrastructure facilities worldwide (mainly synchrotron radiation laboratories).

The candidate is required to hold (or be close to completion) a master's degree in Nanoscience, Physics, Chemistry or related fields.

Reference: PhD/2014/6

Theoretical study of high pressure hydrogen: High temperature superconductor?

Contact: Aitor Bergara (a.bergara@ehu.es) and Ion Errea (ion.errea@ehu.es)

In this project we will apply theoretical ab initio approximations to analyze physical properties of different phases of high pressure hydrogen. Among other things, we plan to characterize their vibrational spectra, both within the harmonic and anharmonic approximations. This will be very helpful to understand the experimental features and identify the experimentally observed structures, which will allow us to understand the eventual metallic transition in high pressure hydrogen, and see if the predicted high temperature superconducting transition occurs. To get this aim we plan to apply and develop new computational approximations to correctly study solid hydrogen.

Reference: PhD/2014/7

Calcium Silicates

Contact: Andrés Ayuela (swxayfea@sw.ehu.es)

We are currently looking for a PhD student in the field of condensed matter physics and first principles calculations to carry research on the phases and nanostructure in calcium silicates present in cements and concrete. This work is in collaboration with a local technological center. Experience in the use of ab-initio electronic structure calculations to study physical properties of condensed matter and to relate them to their chemical composition and atomic structure is preferred. Candidates will be expected to have:

- some experience or strong interest in first principles calculations
- high scientific curiosity towards new research topics

You will work in a stimulating international environment with excellent opportunities for new initiatives and independent research.

Reference: PhD/2014/8

Laser induced cooling in nano-micro structured systems.

Contact person: Joaquín Fernández(joaquin.fernandez@ehu.es)

Optical cryocoolers made of luminescent solids are promising systems for many applications in the fields of optoelectronics, aerospace industry, bioimaging, and phototherapy. To the present day, researchers have used a number of crystals and glass host materials doped with rare-earth ions (Yb³⁺, Tm³⁺, Er³⁺) to yield anti-Stokes optical refrigeration. In these host materials, the attainable minimum temperature is limited by the average phonon energy of the lattice and the impurity concentration. However it has been theoretically demonstrated that cooling efficiency can be dramatically enhanced when the rare-earth-doped material is ground into a powder made of sub-micron size grains. This is caused by two facts: the modification of the phonon spectrum due to the grains finite size and the effects of light localization which may increase the absorptivity.

The present project proposes the study of laser-induced cooling in new nano-micro structures of rare-earth doped sulfide, chloride, and fluoride hosts, with much lower phonon energies than oxide matrices. New nano-micro thermometer devices, based on rare-earth space-resolved spectroscopy of the nano-micro structures, will be developed with the aid of confocal laser multiphoton microscopy to sense the cooling efficiency of these systems. A thorough study of light diffusion in these inhomogeneous structures will also be needed to accomplish this task. Potential applications of these investigations are temperature control managing of photothermal treatments of tumors as well as smart cooling of small electronic devices.

Reference: PhD/2014/9

Theory of electron energy gain spectroscopy and photon-induced near-field electron microscopy.

Contact person: Nerea Zabala (nerea.zabala@ehu.es)

Scanning Transmission Electron Microscopy (STEM) with Electron Energy Loss Spectroscopy (EELS) has become a very accurate tool to study nano-structures by probing the plasmon fields excited by electron probes. In addition to EELS recently an Electron-Energy-Gain Spectroscopy (EEGS) technique has been proposed, which combines the spatial resolution of electron beams and the energy resolution of optical probes. In EEGS, electrons that have absorbed energy from an external light source appear on the negative side of the energy loss spectrum, and the area under an energy-gain peak reflects the response of the sample at the illuminating frequency, thus increasing the energy resolution.

Recently, Barwick et al. (Nature 462, 902 (2009)) developed a time-resolved imaging technique for nano-structures using a femtosecond laser in ultrafast electron microscopy (UEM), the so-called photon-induced near-field electron microscopy (PINEM), increasing the ability to image the plasmon fields by enabling the visualization of the plasmons in optical excitations.

The aim of this PhD project is to develop the theory below these promising techniques and simulate the signals obtained with them for nano-structures of increasing complexity.

A background on classical electrodynamics, quantum physics and computing is required.

Reference: PhD/2014/10

Scanning probe techniques at low temperature.

Contact person: Lucia Vitali (lucia.vitali@ehu.es)

The PhD candidate will join the *Spectroscopy at atomic scale* group at the Material Physics Center. The group focuses its research activity on the understanding of the physical and chemical phenomena occurring at local scale on surfaces. Our main research tools are scanning probe techniques (as scanning tunneling microscopy and spectroscopy as well as atomic force imaging) in ultra-high vacuum at temperatures down to 1 Kelvin.

We are looking for an enthusiastic and self-motivated person able to enjoy scientific research, both working independently as well as in team. He/she will join one of the following projects:

- Formation of organic nanostructures of covalently bonded molecules via on surface chemical reactions
- Formation and characterization of surfaces of topological insulators and of their interfaces with metals or semi-metals
- Formation and manipulation of superconducting structures and interfaces with normal metals.

The successful candidate must have a university background in physics or in chemical physics, holding a master degree. In depth understanding of surface science is desirable. Programming languages (Labview, Matlab) are preferable.

Reference: PhD/2014/11

Optical spectroscopy of quantum dots and semiconductor-metal nanostructures.

Contact person: Yury Rakovich (yury.rakovich@ehu.es)

Withing this project research will be focused on (i) the development of semiconductor nanostructures based on quantum dots, metal nanoparticles and organic molecules for nanoscale optoelectronics and energy conversion devices and (ii) on characterization of these nanostructures by means of various spectroscopic techniques such as absorption and photoluminescence spectroscopy, Raman spectroscopy and fluorescence lifetime microscopy imaging of individual quantum dots and nanostructures. Particular attention will be paid to the investigation of light harvesting processes, energy conversion and transfer in self-assembled nano-systems.

Reference: PhD/2014/12

First-principles description of electronic excitations and plasmonic resonances in nanostructures.

Contact person: Daniel Sánchez-Portal (sqbsapod@ehu.es)

Within the present PhD project we will theoretically study, using first-principles electronic structure calculations, electronic excitations and optical properties (mainly plasmonic resonances) of nano-structured systems. In our studies we will mainly use the so-called time-dependent density functional theory (TDDFT). The intensity and distribution of the electromagnetic field in the neighborhood of nanostructures and inside nanometric cavities will be studied with the aim to apply our results to understand experiments of single-molecule detection by Raman spectroscopy, the enhancement of solar-cell efficiency and the modification of the optical properties of molecules inside plasmonic-cavities (so-called “plexcitons”).