13th of June 2017

MPC
MATERIALS PHYSICS CENTER

CALL FOR PhD STUDENTSHIP

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.

We are currently seeking for bright, highly motivated students who will be able to make the most of this opportunity and take the chance for boosting their visibility and integration within the research community. This is a unique occasion to work in an intellectually stimulating environment in close interaction with all our scientific staff, a wide group of postdoctoral researchers and a large number of international, world-class visitors. There will be plenty of opportunities to develop collaborations and build a global network of contacts of great added value.

Call is open for allocating 3 PhD studentships.

Each studentship will cover a period of three years, including a salary of 17.283,24 € (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 31st December 2017 for the PhD contract to be continued.

Application Process: The following documentation is required for applying:

1. **Updated CV.** Please provide clear contact information.
2. **Brief statement of motivation**, specifying the project you are interested in (see list of available projects below). Only one of the listed projects can be requested.
3. **A letter of acceptance/support** signed by the supervisor of a project is required.
4. **Reference letters** are welcomed but not essential.

Please mind that candidates must choose one project only. Candidatures applying for two or more projects at once will be automatically rejected. All documents must be sent to **mpc@ehu.eus**

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The deadline for this call is 7th July 2017, at 17:00 CEST.

Evaluation Process: Applications will be evaluated by a Committee designated by the CFM Direction Board. The following criteria will be applied:

- CV of the candidate.
- Adequacy of the candidate's technical background to the research topic of the particular project to which he/she is applying for.
- Reference letters.
- Gender Balance.

Only applications received before the deadline (7th July 2017 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.

If you need further information about a specific project, please get in touch directly with the contact person indicated in the project description. For any general queries on the selection process, contact mpc@ehu.eus.

LIST OF AVAILABLE PROJECTS

Project S1. Non-equilibrium effects in nanostructures with spin-dependent fields

Contact person: Sebastian Bergeret (sebastian_bergeret@ehu.eus)
Reference: PhD/2017/1

The thesis will focus on a theoretical study of the electronic transport in hybrid devices with spin-dependent fields. In a first stage of the project the student will be introduced to the technique of the Keldysh Gree's functions and the quantum kinetic equations. These tools will be used in a second stage, when the student will address transport problems related to the coupling between the spin, energy and charge of electrons, as well as the coupling of these degrees of freedom with the electromagnetic environment of realistic devices. The project involved collaboration with experimental groups.

Project S2. Nanoparticles at work: Physics and Chemistry of Curved Crystal Surfaces

Contact person: Enrique Ortega (enrique.ortega@ehu.es)
Reference: PhD/2017/2

Nanocrystals are ubiquitous in chemistry and physics applications. However, technology advances are hampered due to the difficulty to appropriately investigate nanocrystal surfaces at the atomic scale and in-operando conditions (high pressures, high temperatures). We use curved surfaces as model systems to investigate electronic states, chemical activity and structural transformations at the unexplored low-symmetry surface

planes that feature nanocrystals. The work implies the use of Surface Techniques, namely LEED, STM/STS, and electron spectroscopies, such as XPS and ARPES, at both Ultra-High Vacuum and reactive atmospheres (millibar pressure).
The successful candidate should hold a Master Degree in experimental physics or chemistry, dating not before 2014, and have a good background on solid-state physics. The proven ability/experience in Ultra High Vacuum Techniques, plus STM and/or Photoemission experience will be very positively evaluated. The work also involves the use of synchrotron radiation, and hence experience on that will be highly appreciated.
We are looking for a highly motivated candidate, able to work in a dynamic environment and to contribute his/her ideas to the group.

Project S3. Theoretical description of femtosecond laser-induced molecular desorption using abinitio molecular dynamics with electronic friction (AIMDEF) and thermostats

Contact person: Maite Alducin (maite.alducin@ehu.eus)
Reference: PHD/2017/3

Femtosecond laser induced desorption has been experimentally demonstrated to be a promising technique to trigger and control the recombination and reaction of adsorbates on surfaces. However, the complexity and variety of the physical processes involved (electron excitations, surface phonons, adsorbate's excited states) and the strong dynamical nature of all of them have limited our understanding of the variables determining the efficiency and applicability of this technique. The new AIMDEF methodology, which accurately accounts for the electronic and phononic excitations and is also computationally efficient, is perfectly fitted to investigate existing unsolved issues. The objective of the PhD project will be to investigate theoretically, using this methodology, different laser induced desorption scenarios. In particular, to disentangle the mechanisms behind the strong coverage dependence of the desorption yields in the CO/Pd(111) system and the study of systems in which both CO molecular and O atomic adsorbates are present in metal surfaces will be among the milestones of the PhD project. The candidate must have a strong background in condensed matter physics and/or chemical physics. Knowledge in Fortran programming will be also valued.

Project S4. Laser induced cooling in nano-micro structured systems

Contact person: Joaquín Fernández (joaquin.fernandez@ehu.eus) y Rolindes Balda (rolindes.balda@ehu.eus)
Reference: PhD/2017/4

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 [1-6]. 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 [7]. 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, 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.

Project S5. On the structure and dynamics of systems based on single-chain-nanoparticles: atomistic MD-simulations vesus scattering techniques

Contact person: Fernando Alvarez (fernando.alvarez@ehu.es) and Juan Colmenero (juan.colmenero@ehu.eus)
Reference: PhD/2017/5

By analogy to the development experienced in manipulating and visualizing single atoms at the atomic level - giving rise to modern bottom-up nanotechnology - a similar degree of control is expected to become a reality in the future years at the level of individual synthetic polymeric chains for producing functional soft and bio-inspired nano-entities of technological interest, through full development of what is called 'single-chain technology'. In this context, single-chain nano-particles (SCNPs) are polymeric soft nano-objects consisting of uni-macromolecular chains collapsed to a certain degree by means of intramolecular bonding. Sensing capabilities, controlled drug delivery and catalytic applications of SCNPs have been recently demonstrated. Moreover, there is also an increasing interest on SCNPs as components of what are called all-polymer nano-composites, i.e., nano-composites formed by a polymeric matrix and soft SCNPs. In the group of 'Polymers & Soft Matter' of the Materials Physics Center, we are currently carrying out a strong effort to contribute to set the bases of the 'single-chain technology' by means of the study of the processes of formation of SCNPs and the structure and dynamics of soft mater and bio-inspired systems based on SCNPs. In the framework of this project we offer a PhD work based on the combination of classical molecular dynamics simulations at atomistic level with scattering techniques – a synergetic combination which has proven to be an invaluable tool to investigate polymer based materials.

The proposed PhD project will focus on the following workpackages:

1) Study by atomistic MD-simulations combined with X-ray and neutron scattering of the structure and dynamics of polymer precursors of SCNPs in solution and bulk.

2) Development of atomistic MD-simulation methods to investigate the process of formation of SCNPs by intramolecular cross-linking
3) Study by atomistic MD-simulations combined with neutron and X-ray scattering of the structure and dynamics of SCNPs in solution and bulk conditions.

Project S6. Molecular dynamics of polymer systems by fast scanning calorimetry and dielectric spectroscopy

Contact person: Daniele Cangialosi (daniele.cangialosi@ehu.eus)
Reference: PHD/2017/6

The present project aims to exploit the potentiality of fast scanning calorimetry (FSC) to determine molecular dynamics. This technique allows measuring the temperature dependent specific heat over heating/cooling rate as large as several thousands Kelvin/seconds. Through appropriate thermal protocols, FSC delivers information on the molecular dynamics on a broad time scale range, including milliseconds. This characteristic makes FSC a technique complementary to the widely used broadband dielectric spectroscopy. The latter, while covering a wide range of time scales, presents a number of drawbacks including the inability to provide information on the molecular mobility of systems with negligible dipole moment or those where conductivity related processes hide crucial information on the molecular mobility. The project is therefore focused on the connection of the calorimetric response with the dielectric relaxation data for a number of relevant systems in soft matter science, including polymer blends and other heterogeneous/multicomponent polymer systems.

Project S7. On surface chemical reactions

Contact person: Lucia Vitali (lucia.vitali@ehu.eus)
Reference: PhD/2017/7

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.
We are looking for an enthusiastic and self-motivated person able to enjoy scientific work working independently as well as in team. He/she will join the project called “On surface chemical reactions”.
Aim of this work is to investigate new chemical reaction processes leading on one side to molecular polymerization on surfaces and on the other to create functional surfaces to promote catalytic reactions. Here, we aim to explore the viability of the synthesis of these structures and their functionality using scanning microscopy, atomic force imaging and spectroscopy techniques in ultra high vacuum at temperatures down to 1Kelvin. The surface preparation and characterization will be done in UHV.

The successful candidate has a university background in physics or in chemical physics, and a depth understanding of surface science. Programming languages (Labview, Mathlab) are preferable.

Project S8. Looking for new fermions in conventional crystals

Contact person: Aitor Bergara (a.bergara@ehu.eus) and Maia Garcia Vergniory (maia.garcia@ehu.eus)
Reference: PhD/2017/8

Very recently Bradlyn et al. (Bradlyn et al. Science 353 (6299)) suggested that non symmorphic crystals can show a new family of topologically protected fermionic quasiparticles. In this work we plan to apply chemical/physical topology to find ideal materials with such interesting properties.

Project S9. From single-chain nanoparticles to gels: Computational study of the competition between intra- and inter-molecular bonding of polymers in solution

Contact person: Angel J. Moreno (angeljose.moreno@ehu.eus)
Reference: PhD/2017/9

The aim of this PhD project is to investigate, by using molecular dynamics and Monte Carlo simulations, the phase behavior of solutions of functionalized polymers that can form both intra- and inter-molecular bonds. The possibility of forming, among others, single-chain nanoparticles, monodisperse clusters, reversible and irreversible gels, will be systematically investigated as a function of the concentration and polymer characteristics (architecture, homo/heterofunctionality, amphiphilicity, etc).

We are looking for a motivated candidate fulfilling the following requirements:

1) Background in soft matter science.
2) MSc degree in Physics, Chemistry or related fields, or expected to obtain it within next months.
3) Experience in molecular dynamics and/or Monte Carlo simulations.

Project S10. Engineering of two dimensional materials properties through atomic defects

Contact person: Martina Corso (martina.corso@ehu.eus) & Sara Barja (sara.barja@ehu.eus)
Reference: PhD/2017/10

The properties of two-dimensional (2D) materials are highly sensitive to the presence of defects and a detailed understanding of their structure may lead to the emergence of novel physico-chemical functionalities through “defect engineering”. Defects characterization at the atomic level has been extensively done on graphene. Similar studies have not been performed exhaustively on 2D Transition Metals Dichalcogenides and hexagonal boron despite the exciting modification of their electronic, magnetic and catalytic properties predicted

theoretically. The aim of this project is to directly correlate the atomic and electronic structure of defects in two dimensional materials and identify their role in the fundamental material properties.
Two dimensional materials will be grown in ultra-high vacuum by molecular beam epitaxy (MBE) or chemical vapor deposition (CVD) and studied by surface sensitive techniques as Scanning Tunneling Microscopy at low temperatures and X-ray photoelectron spectroscopy.

Project S11. Dynamics and structure of ice in anti-freeze and ice nucleation proteins.

Contact person: Silvina Cerveny (silvina.cerveny@ehu.es)
Reference: PhD/2017/11

Ice-binding proteins (antifreeze proteins (AFPs)) aid the survival of freeze-avoiding organisms by inhibiting the growth of ice crystals. By contrast, an ice nucleation protein (INP) increases the ability to form ice. In this thesis, we propose to study the structure and dynamics of ice in presence of both AF and IN proteins by combining Electron Microscope and broadband dielectric spectroscopy (BDS). Studies will be performed on a broad range of concentrations from well-diluted to concentrate solutions. Proteins will be selected to obtain different quaternary structures to explore the influence of the shape on nucleation properties as well as the influence of the local chemistry of the surfaces (hydrophobic-hydrophilic). The main goal of this project is to find a common mechanism of proteins for binding ice. This thesis will be performed in a close collaboration between the Material Physics Center and Nanogune.