13th of June 2017

MPC
MATERIALS PHYSICS CENTER

CALL FOR POSTDOCTORAL POSITIONS

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 young researchers 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 2 Postdoctoral appointments.

Each position will cover a period of two years (1+1, with renewal for the second year subject to evaluation of performance). The salary will be 34.021,20 € per year (before taxes). Funding is provided by the Research Association MPC – Materials Physics Center.

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 scientific background to the position to which he/she is applying.
- Reference letters.
- Gender balance and opportunities to young researchers.

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.es.

LIST OF AVAILABLE PROJECTS

Project P1. Nanoparticles at work: Physics and Chemistry of Curved Crystal Surfaces

Contact person: Enrique Ortega (enrique.ortega@ehu.es)
Reference: PD/2017/1

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, electrochemical cells). 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 three-dimensional nanocrystals.

The work implies the use of a full battery of Surface Techniques, namely STM and electron spectroscopies, such as XPS and UPS, at both Ultra-High Vacuum and reactive atmospheres (millibar pressures and electrolytes). The successful candidate should hold a Doctoral 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 P2. Dynamics of the CO-O recombination at metal surfaces studied from first principles

Contact person: Joseba Iñaki Juaristi (josebainaki.juaristi@ehu.eus)
Reference: PD/2017/2

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 addition, these processes usually being highly exothermic, they are also known to be a major source of surface damage in general plasma-wall interactions, such as those occurring on the internal walls of fusion reactors or on aerospace vehicles during the atmospheric entry. 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 the coverage. The objective will be to determine the surface electronic properties that cause such a dependence. The candidate should hold a PhD in theoretical or computational physics or chemistry and must have a strong background on density functional theory, as well as, high expertise in computational work. Experience on gas-surface dynamics simulations will be also valued.

Project P3. Scanning probe techniques at low temperature

Contact person: Lucia Vitali (lucia.vitali@ehu.eus)
Reference: PD/2017/3

The post-doctoral candidate will join the Spectroscopy at atomic scale group at the Centro de Fisica de Materiales. The group research interests aim to understand of 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.

The present project aims to exploit and further develop one of the following topics:

- Chemical reactivity on two dimensional surfaces
- On-surface polymerization of organic molecules leading to the formation of covalently bonded organic structures on different substrates.

The successful candidate has a degree in physics or chemistry and has experience in scanning tunneling spectroscopy in ultra-high vacuum environment. Knowledge of low temperature physics and programming languages (Labview, Mathlab) are preferable. We are looking for an enthusiastic and self-motivated post-doctoral person able to enjoy scientific work working independently as well as in team.

Project P4. Dynamics of elementary reactive processes at surfaces

Contact person: Ricardo Díez Muiño (rdm@ehu.eus)
Reference: PD/2017/4

Advances in the description of elementary reactive processes at surfaces are largely triggered by the quest for systems and conditions under which reactivity can be controlled, enhanced or inhibited. From this point of view, two-dimensional (2D) layered systems, such as transition metal dichalcogenides or transition metal carbides/nitrides, are receiving increasing attention due to their high activity as catalytic agents. The catalycity of these systems can be also very dependent on the presence of defects as well as on the nanostructural properties when the system is finite (nanoribbons, nanosheets, etc.). The goal of this project is to advance in the theoretical description of physico-chemical processes that involve the interaction between small molecules (H2, N2, O2…) and 2D materials. Ab-initio molecular dynamics (AIMD) based on density functional theory (DFT) will be used to describe the dynamics of adsorption and dissociation processes. Candidates to this position must hold a PhD degree in physics or chemistry and should have experience in first-principles theoretical methods as well as in numerical simulations.

Project P5. Coarse-grained molecular dynamics simulations of soft nanoparticles as stabilizers for Pickering emulsions

Contact person: Angel J. Moreno (angeljose.moreno@ehu.eus)
Reference: PD/2017/5

The aim of this postdoc project is to investigate, by using molecular dynamics simulations at different levels of coarse-graining (from bead-spring models to ultrasoft single-particles), the structural and thermodynamic properties of polymer-based soft nanoparticles at liquid-liquid interfaces, as well as the potential use of these soft nano-objects for stabilizers of Pickering emulsions. The simulated soft nanoparticles will be, among others, single-chain nanoparticles, star polymers and dendrimers.

We are looking for a motivated candidate with a high expertise in computer simulations of soft matter systems. The candidate must hold a PhD degree or be expected to get it within next months.

Project P6. Ultra-dense/low energy state glasses by aging nanostructured polymers

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

This project takes inspiration from recent findings showing that glasses exhibiting large amount of free interface are able to access low energy states in remarkable short time scales. Hence, the thermodynamic state in these kinds of glasses – including polymer nanospheres, nanocomposites, thin films and foams – subjected to different thermal histories will be characterized. To do so, we plan to employ conventional and fast scanning calorimetry, that is, techniques providing access to the enthalpy state of a given glass. Complementary techniques, such as broadband dielectric spectroscopy, will also be used. Exploring low energy states will allow producing ultra-dense glasses. This may result in a tremendous impact on the glass properties. Apart from this, the present project aims to clarify long-standing fascinating issues of glass science, such as the existence of the so-called "ideal" glass, that is, a disordered system with entropy equal to that of the corresponding ordered crystal.

Project P7. Optical response and plasmon propagation in nanostructures based on novel materials

Contact person: Nerea Zabala (nerea.zabala@ehu.eus)
Reference: PD/2017/7

This postdoctoral position will target theoretical and numerical research on nanoscale photonics. The main goal of this project is to describe surface plasmon excitation and propagation in different nanostructure designs containing metallic, ferroelectric and magnetic materials.

We are looking for a post-doctoral candidate with expertise in theoretical and computational electrodynamics to address the optical response of plasmonic nanoantennas and nanostructures of novel materials of technological interest.

Experience in numerical methods to solve Maxwell equations and use of FDTD (Finite Difference Time-Domain) codes is required for this position. A strong theoretical background in photonics and condensed matter physics is also a prerequisite. An interacting attitude towards group working is also highly desirable.

The candidate will be a motivated researcher with a PhD degree in Physics and with expertise in computer simulations.

Project P8. Graphene Nanoribbons nanotechnology: coupling graphene nanoribbons to insulators and gateable systems

Contact person: Martina Corso (martina.corso@ehu.eus)
Reference: PD/2017/8

Graphene nanoribbons (GNRs) technology is still in its infancy and a few problems need still to be solved to speed up their use in current technology. For their operation in devices, as in gated multiterminal devices, GNRs have to be transferred to insulators. The aim of this project is to find effective routes to directly grow or transfer GNRs to insulating surfaces and characterize their electronic and structural properties afterword. Different strategies will be used as: alternative reactions to Ullmann Coupling for on-surface synthesis, polymerization induced by light, intercalation, or transfer of GNRs by atomic layer injection. The candidate will work with several surface sensitive techniques as Angle Resolves Photoemission (ARPES), Scanning Tunneling Spectroscopy (STM) and X-Ray Photoelectron Spectroscopy (XPS) in ultra-high-vacuum to define the coupling between GNRs and the insulating substrate with atomic precision.

Project P9. Theoretical studies of isolectronic compounds to graphene and phosphorene

Contact person: Andres Ayuela (swxayfea@sw.ehu.es)
Reference: PD/2017/9

New phenomena in condensed matter physics are based on two-dimensional materials.

Although graphene looks promising for the future, research is today focusing on other carbon nanostructured materials and other two-dimensional materials.

The possibility to exfoliate materials and the existence of accurate experimental tech- niques to study single-layer materials supposed a big boost to study other layered ma- terials. Layers with other elements in the carbon group have been studied to produce coun- terparts to graphene, such as silicene, germanene or stanene. Graphene is flat because there is sp2 hybridization, and these other compounds adopt a buckled structure because they prefer sp3 hybridization. Other layered nanostructures isoelectronic to graphene must be considered using density functional calculations.

Phosphorene has also a two dimensional honeycomb puckered structure where each atom is bonded to three neighbors. It displays a direct band gap, tunable attending to the number of layers the stacking. We are also going to consider phosphorene isoelectronic compounds and attending to the number of layers we would have to study the eletronic and optical properties.

Project P10. Bulk photovoltaic effect from first-principles using Wannier functions

Contact person: Ivo Souza (ivo_souza@ehu.es)
Reference: PD/2017/10

The bulk photovoltaic effect (BPVE) is a nonlinear optical response that yields a net photocurrent in noncetrosymmetric crystals. Contrary to the photovoltaic effect occurring in pn junctions, the BPVE is able to generate an above band-gap photovoltage, making it an attractive alternative to conventional solar cells. From a more fundamental perspective, it has been suggested that the BPVE may provide a "smoking-gun" transport signature of the nontrivial band topology in Weyl semimetals, a newly-discovered class of topological meterials.

Although the theory of the BPVE is well established, its practical implementation is challenging. In particular, the expression for the "shift-current" contribution in polar materials involves a subtle Berry-phase-like quantity. Because of such issues, ab-initio calculations of the BPVE are still in their infancy.

The goal of the project is to develop and implement a practical and efficient ab-initio methodology for calculating the BPVE using localized Wannier functions, and to apply it to Weyl semimetals and other materials of current interest.