

## 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 3 Postdoctoral appointments.

Each position will cover a period of two years (1+1, with renewal for the second year subject to evaluation of performance), starting date would be January 2020. The salary will be 34.642, 20€\* per year (before taxes). Funding is provided by the Research Association MPC – Materials Physics Center.

\*In the previous publication there was an error with the advertised gross salary. Sorry for any inconvenience

**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 [jobs.cfm@ehu.eus](mailto:jobs.cfm@ehu.eus)

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**The deadline for this call is 4<sup>th</sup> November 2019, at 12:00 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 (4<sup>th</sup> November 2019 at 12:00 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](mailto:mpc@ehu.es).

## LIST OF AVAILABLE PROJECTS

### **Project P1. Interaction of quantum states of light with nanostructures at low temperatures.**

*Contact person: Gabriel Molina Terriza (gabriel.molina.terriza@gmail.com)*

*Reference: PD/2019/1*

The post-doctoral candidate will join the Quantum Nanophotonics Laboratory at the Centro de Física de Materiales. The research group focuses on studying the interaction of light and matter at the nanoscale, with applications to quantum technologies and nanophotonics. In particular, we are interested in developing a new class of quantum-enhanced sensors for measuring acceleration, magnetic fields and improving imaging techniques for nanophotonics.

The aim of this project is to investigate the interaction between engineered quantum states of light, such as entangled photon states and quantum squeezed states of light, with nanostructures. Our laboratory is fully equipped for quantum optics experiments and we host an optically addressable cryostat in order to control the temperature of our samples. We aim to control the quantum properties of plasmonic and dielectric structures with quantum light.

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The successful candidate should have a PhD in physics or engineering, and experience in the development and control of quantum sources of light or in nanophotonics experiments. Knowledge on the operation of closed cycle cryostats and Python programming will also be valuable.

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### **Project P2. Transport Properties of Ising and Rashba superconductors.**

Contact person: Sebastian Bergeret ([sebastian\\_bergeret@ehu.es](mailto:sebastian_bergeret@ehu.es))

Reference: PD/2019/2

The post-doctoral candidate will join the Mesoscopic Physics Group (MPG) at the Centro de Física de Materiales. The MPG is a theory group with a main research focus on transport properties of nanostructures, superconductivity and magnetism. In past years the group has been predicted several novel effects with direct applications in spintronic, caloritronics and electromagnetic sensing (for details see <https://cfm.ehu.es/mesoscopics/>).

The aim of this project is to explore properties of two-dimensional superconductivity in systems with strong spin-orbit coupling (SOC) and to develop new theoretical tools for the studies. Specifically, we envision two different approaches for the investigation depending on the type of superconductivity: For Rashba SOC we will extend the covariant SU(2)-covariant formalism developed in the MPG during the past years for finite systems in out-of-equilibrium situations. For superconductors of ionic type the plan is to develop a quasiclassical theory that allows the study of transport properties in systems with hybrid boundaries, interfaces, and disorder. Collaboration with local experimental groups is also planned.

The successful candidate should have a PhD in Physics, good theoretical skills in both analytical and numerical methods in Condensed Matter Physics, and basic knowledge of superconductivity and non-equilibrium physics.

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### **Project P3. Dynamics of molecules interacting with 2D systems.**

Contact person: Ricardo Diez Muiño ([rdm@ehu.es](mailto:rdm@ehu.es))

Reference: PD/2019/3

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 catalytic activity of these systems can be also very dependent on the presence of defects as well as on the Nano structural 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

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molecules (H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>...) 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.

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**Project P4. Theoretical description of femtosecond laser-induced molecular desorption and reactivity.**

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Contact person: Maite Alducin Ochoa ([maite.alducin@ehu.eus](mailto:maite.alducin@ehu.eus))

Reference: PD/2019/4

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 that accurately accounts for the electronic and phononic excitations and is computationally efficient is perfectly fitted to investigate existing unsolved issues. The objective of the project will be to investigate, 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. 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.

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**Project P5. Dynamics of the CO-O recombination at metal surfaces studied from first principles.**

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Contact person: Joseba Iñaki Juaristi Oliden ([josebainaki.juaristi@ehu.eus](mailto:josebainaki.juaristi@ehu.eus))

Reference: PD/2019/5

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

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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.

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**Project P6. Computer simulations of transport of soft nanoparticles in nanocomposites and polymeric networks.**

Contact person: Angel Moreno ([angeljose.moreno@ehu.es](mailto:angeljose.moreno@ehu.es))

Reference: PD/2019/6

Dispersion of nanoparticles in polymer matrices is an efficient way to design hybrid polymer-based materials. A novel alternative to decorated hard nanoparticles is to use fully polymeric nanoparticles with the chemistry of the matrix, leading to "all-polymer nanocomposites". Because these nanoparticles are fully penetrable, the usual separation between confinement and entanglement effects vanishes. Most of the investigations on the rheology of nanocomposites have focused on the chain dynamics of the matrix, using the framework of the tube model, where the entangled chains relax through reptation in an effective tube modified by the presence of the nanoparticles. Much less is known about the transport properties of the nanoparticles. A crossover from free diffusion to hopping has been found by increasing the nanoparticle size above the tube diameter. However, such studies are limited to the case of hard nanoparticles, for which penetration by the chains is not possible. In this project, we aim to obtain a general scenario for the transport of soft penetrable nanoparticles in nanocomposites and networks. We will simulate the dynamics of single bead-spring nanogel-like and star-like nanoparticles in polymeric networks, using as control parameters the softness of the nanoparticle and the mesh size. The candidate should have a solid background in soft matter physics and experience in computer simulations.

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**Project P7. Theory of electronic, topological and magnetic properties of covalent molecular networks.**

Contact person: Daniel Sánchez Portal ([daniel.sanchez@ehu.es](mailto:daniel.sanchez@ehu.es))

Reference: PD/2019/7

The post-doctoral candidate will join the Group of Modelization and Simulation at the Centro de Física de Materiales.

We will investigate the electronic and transport properties of covalent molecular networks (CMNs), mostly graphene nanoribbons (GNRs) first-principles DFT and tight-binding calculations and the non-equilibrium Green's function formalism:

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- In relation with STM experiments developed at nanoGUNE in which the CMN is contacted and lifted by the tip, giving access to the properties of free-standing CMNs and shedding light into the influence of the interaction between the CMNs and the underlying substrate. Chemically doped armchair GNRs and chiral GNRs will be investigated.

- In relation to two-probe scanning tunneling spectroscopy experiments performed by Dr. M. Kolmer at Oak Ridge Nat. Lab. (USA) we will study the electronic transport along zigzag-edge sidewall GNRs grown on 6H-SiC{11-2n} facets [Mie19]. This system shows remarkable ballistic transport over distances of hundreds of nanometers that remain unexplained.

- Topological properties of GNRs of arbitrary chiralities will be explored in an attempt to understand their magnetic properties.

The successful candidate should have a PhD in physics or chemistry, and experience in first-principles electronic structure calculations.

### **Project P8. Electronic Properties of Van der Waals Graphene Nanostructures.**

Contact person: Andrés Ayuela ([swxayfea@sw.ehu.es](mailto:swxayfea@sw.ehu.es))

Reference: PD/2019/8

The post-doctoral candidate will join the Group of Electronic Excitations in Surfaces and Nanostructures at the Centro de Física de Materiales, mostly devoted to the theoretical study of electron dynamics in solids, surfaces, nanoscale systems and materials of technological interest. Furthermore, the research group focuses on studying electronic and magnetic properties of materials mainly using first principles methodologies. This topic is of high interest in the area of advanced materials, such as Van der Waals two-dimensional nanostructures.

In this project, we aim to study the electronic properties of graphene-based heterostructures, for instance, bilayers and bilayer flakes. We will study topological states in carbon-based systems, when grain boundaries and deformations are included. We will look at the interplay of localized states of different origins, such as related to edges due to vacancies, ad-atoms and defects, with the topologically protected states, which behave as one-dimensional conducting channels.

This work mainly requires the use of tight binding methods, and the proven ability/experience in tight binding codes will be very positively evaluated. Although some experience in methods within density functional theory would also be appreciated.

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### **Project P9. PRESSURE INDUCED TOPOLOGICAL TRANSITIONS.**

Contact person: Aitor Bergara ([a.bergara@ehu.es](mailto:a.bergara@ehu.es))

Reference: PD/2019/9

The post-doctoral candidate will join the Quantum Theory Group at the Centro de Física de Materiales. The research group focuses on analyzing the physical properties of different materials within the Density Functional Theory.

The aim of this project is to investigate the pressure induced topological transitions in simple systems (e.g. hydrogen, hydrogen rich alloys and alkalies) and their eventual relation with superconductivity.

A number of exotic phenomena arise under high pressure. For example, pressure enhances the superconducting transition temperature. Actually, LaH10 super conducts at 260 K and 200 GPa, becoming the highest T<sub>c</sub> ever measured. On the other hand, topologically non-trivial materials have become a hot topic in recent condensed matter physics research. In this PhD Project, we propose to analyze possible pressure induced topological transitions even in simple systems, as a result of the already observed enhanced electronic complexity under pressure. The study of the eventual connection between the topological transition and superconductivity will also be part of the research project.

The successful candidate should have a PhD in physics or chemistry, and experience in Density Functional Theory calculations.

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### **Project P10. Polymer structure and dynamics: comparing 3D polymer networks obtained from polymer chains of different topologies.**

Contact person: Angel Alegria ([angel.alegria@ehu.es](mailto:angel.alegria@ehu.es))

Reference: PD/2019/10

The post-doctoral candidate will join the Polymer and Soft Matter Group (PSMG) at the Centro de Física de Materiales. The research group mainly focuses on studying the structure and dynamical properties of polymer-based soft-matter. A general overview of the activity developed during the last years can be found at <http://www.sc.ehu.es/sqwpolim/PSMG>.

One of the topics the group is deeply involved over the last few years is the investigation of the effect on the structure and dynamics of the intra-chain bonding-giving rise to the collapse of the individual single linear chains of a polymer.

The aim of the present project is to compare in detail how this single chain collapse influences the properties of the materials obtained by a subsequent inter-chain bonding, which results in a 3D polymer network. It is anticipated that the rheological properties of this kind of material

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are going to be markedly different from those of the corresponding 3D polymer network obtained without a previous intra-chain collapse.

Differences are also expected at the level of the molecular motions involving a few repeating units (segmental dynamics), which are of utmost importance for applications. To explore the relevance of the different topologies on the properties of the resulting 3D network polymer, similar materials obtained by inter-chain bonding of cyclic chains will be also investigated.

The successful candidate should have a PhD in physics, chemistry, or related topics, and experience in the basic experimental techniques for polymer investigation, and particularly on scattering and relaxation methods.

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### **Project P11. Surveying chemical reactions and interface properties at surface.**

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

Reference: PD/2019/11

The post-doctoral candidate will join the Group of *Spectroscopy at atomic scale* at the Centro de Física de Materiales (<https://cfm.ehu.es/atomic-spectroscopy/>). The research group focuses on the characterization of surface phenomena occurring at atomic and sub-molecular scale aiming to understand the correlation between adsorption geometry, electron density of states and chemical reactivity.

Within this project, the postdoctoral candidate will be involved in one or more of the following topics, where the node is the local spectroscopic characterization:

- Metal-organic interactions involving chalcogen atoms and/or alkali atoms
- Chemical reactions promoted either electro induced or catalyzed by the supporting surface.

The successful candidate should have a PhD in physics or chemistry, or physics, and demonstrated experience in low temperature scanning probe techniques.

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### **Project P12. Bridging the gap between the dynamics of synthetic polymers and biopolymers.**

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Contact person: Silvina Cerveny ([silvina.cerveny@ehu.es](mailto:silvina.cerveny@ehu.es))

Reference: PD/2019/12

The general framework of this project is to contribute to the understanding of the dynamics of bio-macromolecules, such as proteins and peptides, in aqueous environments with and without the presence of ice. We are currently running a project focused on the differences and similarities between the dynamics of aqueous solutions of synthetic polymers and polymers with biological activity. On the other hand, we also studied the ice generation in diluted solutions of ice nucleation proteins that can be considered as soft bio-nanoparticles. The aim of the present project is to contribute to set the bases to close the gap between polymers and biopolymers by means of the study of the structure and dynamics of soft matter.

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The present project will be based on the application of dielectric techniques to analyze the dynamics as well as other characterization techniques such as environmental SEM, SAXS, FTIR, etc.

The post-doctoral candidate will join the Group of Polymers and Soft Matter at the Centro de Física de Materiales. The successful candidate should have a PhD in physics or chemistry and experience in dielectric techniques. Knowledge on biopolymers is also acknowledged.

### **Project P13. Polymerization on unconventional surfaces.**

Contact person: Celia Rogero ([celia.rogero@ehu.eus](mailto:celia.rogero@ehu.eus))

Martina Corso ([martina.corso@ehu.eus](mailto:martina.corso@ehu.eus))

Reference: PD/2019/13

The Nanophysics Laboratory of the Materials Physics Center (CFM-MPC) in San Sebastian, Spain, has an opening Postdoctoral position in Experimental Surface Science.

The research topic will be “physico-chemical aspects of surfaces”. The work will consist on exploring and designing new molecular complexes directly synthesized on surfaces in order to provide ground ideas for functional devices of various nature. The aim is to characterize and understand the bases of the functional phenomenology of molecular materials synthesis on substrate with interest for future technological devices, such as electronics, magnetic storage or optoelectronic deceives.

Since most of the work will be performed in ultray high vacuum (UHV) conditions, the candidate should have proven experience in ultra-high vacuum and in some of the surface science characterization techniques (STM, AFM, XPS, synchrotron radiation...). Previous experience with surface science techniques will be desirable. We are looking for highly motivated candidates, able to work in a dynamic environment and to contribute with his/her own ideas to the group.

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