CALL FOR PhD STUDENTSHIP

The Center for Materials Physics (CFM) in Donostia / San Sebastián (the Basque Country, Spain) is currently seeking for bright, highly motivated PhD candidates. The successful students will work in an intellectually stimulating environment to develop cutting-edge research on Materials Science, exploring physical and chemical properties of advanced materials, nanostructures and nanodevices, either theoretically or experimentally.

They will have access to the most advanced techniques in the field and develop industry-transferable skills. The PhD candidate will work in close interaction with all our scientific staff and a wide group of postdoctoral researchers, and will take advantage of a continuous flow of prestigious international visitors. CFM is a joint center of the University of the Basque Country - UPV/EHU and the Spanish Research Council - CSIC. The center brings together several research teams with international recognition and positioning, developing cutting-edge materials science in state-of-the-art facilities.

CFM's headquarters are located in Donostia / San Sebastián, a vibrant city on the northern coast of Spain, featuring an intense cultural life (including international cinema and jazz festivals) and an extraordinary natural landscape. Donostia is a unique place to conduct research, as it concentrates several world-leading research centers, such as the CFM, the Donostia International Physics Center (DIPC), the CIC Nanogune or the CIC Biomagune, among others.

The successful candidates will benefit from an environment that fosters the cross-fertilization of ideas between different research topics. This year, the CFM is focused on the following research projects[1]:

Project S1. Biophysics of potassium channels: from atomistic protein folding, to clinical testing and drug design

Project S2. Greenhouse gas sequestration at the atomic scale: dry reforming of methane molecular beams

Project S3. Magnetism meets superconductivity

Project S4. Spin-vibration coupling in magnetic impurities

Project S5. Development of biodegradable adsorbents for the removal of emerging contaminants (pesticides, pharmaceuticals and heavy metals) from water

Project S6. First-principles analysis of the charge-density wave transitions in Kagome topological superconductors

Project S7. Moiré quantum matter in 2D-materials characterized by local spectroscopic techniques

Project S8. PhD in experimental surface electrochemistry 2D materials for water electrolysis.

Project S9. Tuning the Assembly of Proteins in Lipid Bilayers

The candidates are expected to work in these areas. More details on these research lines can be found in our web page: https://cfm.ehu.es/research-lines

4 PhD studentships available

We will follow an online selection process. The details will be defined and published in CFM's website and will include interviews and discussions with the supervisor of the different research projects and/or the Evaluation Committee.

From the interviews, four (4) candidates will be selected and granted full studentships. Each studentship will cover a period of three years, including a salary of 17.398,20 € (before taxes) during the first year, with subsequent increases of around plus 1000 euros per year, over the following two years. The studentship will also include a budget (allocated to the research group) covering research and training expenses. The PhD studentship will only be granted to successful candidates whose PhD project will be formally registered at the University of the Basque Country

[1] *Please mind that candidates can choose a maximum of 4 projects.*

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UPV/EHU before 31st December 2023 for the PhD contract to be continued. Therefore, **the candidates are required to hold a Master degree granted before the end of 2023**.

Application Process: Find all the necessary information about how to apply, as well as future updates and publications here: https://cfm.ehu.es/education/phd-recruitment-fair/

The following documentation is required for applying:

1. Fill in relevant data in the on-line form.
2. **Updated CV.** Please provide clear contact information.
3. **Reference letters** (if more than one, please merge all of them in a single e-file).

The deadline for the application is 31st May 2023, at 13:00 Central European Time (CET)[2].

Pre-Selection Process: The applications will be evaluated by an academic Evaluation Committee composed by permanent CFM faculty members, who will consider the CVs of the candidates, the adequacy of their background to the selected projects and the provided reference letters.

Pre-Selection Results: All candidates will be notified of the results by email and the pre-selected candidates will be contacted personally for arranging the calendar of the on-line interviews with the different research-project supervisors and/or the Evaluation Committee.

Final Selection Process: Soon after the on-line interviews, the committee will select the 4-awarded students and the final decision will be communicated to the applicants and published in the CFM website (http://cfm.ehu.es/about-cfm/job-offers).

If you need further information about this call or about any general queries on the selection process, please contact phdstudents.cfm@ehu.es

[2] *Only applications received before the deadline (31st May 2023 at 13:00 CET) will be evaluated.*

LIST OF AVAILABLE PROJECTS

Project S1. Biophysics of potassium channels: from atomistic protein folding, to clinical testing and drug design

Contact person: Aitor Bergara (a.bergara@ehu.eus) and Aritz Leonardo (aritz.leonardo@ehu.eus)

The Kv family of ion channels are tubular-shaped proteins allocated in the membrane of neurons. These proteins control the traffic flow of potassium ions between the inside and outside of the cell, and hence, electrical communication between neurons and muscles. Mutations occurring on the Kv channels have been linked to different subtypes of epilepsies. Moreover, it is unclear why or how motor neurons die in amyotrophic lateral sclerosis (ALS), yet we do know that the activity of these channels is altered and that these dying cells undergo spontaneous (uncontrolled) electrical discharges. Hence, defects in ion channels may cause these motor neurons to degenerate. A drug named Riluzole that fits into a specific pocket of the potassium ion channels alters how they work, and is the first approved treatment for ALS. The present project is multidisciplinary and has the following objectives:

- Perform Molecular dynamics simulations to support the hypothesis that certain mutations cause erroneous cotranslational folding of the channel inside the Ribosome.
- Extend the algorithm developed by our group based on Machine Learning intended for clinical use, which correctly predicts the pathogenicity of possible mutations that occur in these proteins.
- In-silico repurpose approved molecule libraries, that resemble the effect of Riluzole on the channels.

It is not necessary for the candidate to have previous knowledge of biology, but he/she must like computing.

Project S2. Greenhouse gas sequestration at the atomic scale: dry reforming of methane molecular beams

Contact person: Enrique Ortega (enrique.ortega@ehu.eus)

Sequestration and recycling of greenhouse gases (GHGs) has become one of the greatest environmental challenges. One straightforward solution is the reforming of methane with carbon dioxide, called dry reforming of methane (DRM), which converts the two main GHGs (CO_2 and CH_4) into syngas (H_2+CO), essential ingredient to produce organic fuels. Our Project aims at studying the DRM process with atomic/molecular scale detail, by monitoring the interaction of a monochromatic CH_4 molecular beam with a CeO_2 catalyst surface immersed in CO_2 gas. The first goal is to assemble and test a unique experimental system, which combines a micron-focused molecular beam setup [1], with an X-ray photoemission (XPS) system. The final objective is to optimize the DRM process over a nanostructured CeO_2(111) surface, tuning the CH_4 beam

properties (energy, scattering angle) and the density/type of active surface sites (atomic steps, kinks), while continuously probing chemical species at the catalyst surface (XPS) and at the gas phase. The project is a joint effort of the Surface Science group at the Universidad Autónoma de Madrid and the Nanophysics Lab-Green Chemistry group at the Centro de Física de Materiales (CSIC/UPV-EHU) [2].

[1] *Diffraction of CH_4 from a Metal Surface,* J. Phys. Chem. Lett. **10**, 1574 (2019).

[2] https://cfm.ehu.es/nanophysicslab/

Project S3. Magnetism meets superconductivity

Contact person: Nicolas Lorente (nicolas.lorente@ehu.eus) and Deung-Jang Choi (djchoi@dipc.org)

Superconductivity takes places when electrons pair leading to a small region of energy about the Fermi energy where no single electron can be injected. As a consequence, there is a gap in conductance measurements near zero bias. However, impurities (atomic or molecular) can weaken and eventually destroy the pairing of electrons. New electronic states appear in the gap. Since these are single-electron states, tunneling from a nearby electrode (such as in the case of the scanning tunneling microscope (STM)) can take place leading to a measurable current and conductance. Depending on the type of adsorbate or impurity and on the type of superconductor, the in-gap states show different properties. As the number of impurities increase, the in-gap states evolve into bands and the topology of these bands can lead to zero-energy states at the border of the atomic structure. These edge states are called Majorana bound state. They are exotic in that when exchanged a non-trivial unitary transformation takes place and they are at the origin of Topological Quantum Computation. The object of this thesis work is to perform theoretical and experimental studies using surface techniques to characterize and explore the above physics.

Methodology

This thesis work is a joint theoretical and experimental effort. Experimentally, the work will be to perform STM studies of atomic and molecular adsorbates on superconducting surfaces, use the STM's atomic manipulation capabilities to create nanostructures and use the tunneling and contact regimes of the STM to explore the tunneling of electrons and Cooper pairs in these systems. Other type of surface science measurements will also be performed to complete the STM data. In particular synchrotron studies of X-ray Dichroism can be fundamental to access the inner magnetic moment distribution of the adsorbed systems. Theoretical studies will try to rationalize the experimental findings. The Bogoliubov-de Gennes (BdG) equations will be implemented to study different type of superconductors and different types of impurities. The

solution of the BdG equation in different regimes should yield a direct comparison with the experimental data, permitting us to access the physical phenomena at work.

Project S4. Spin-vibration coupling in magnetic impurities

Contact person: Maria Blanco (maria.blanco@ehu.eus) and Asier Eiguren (asier.eiguren@ehu.eus)

The zero-dimensional limit of a magnet can be realized in organic molecules featuring a magnetic atom center and in adatoms on surfaces. Although both 3d and 4f atomic species can be used, the latter shows more advantages, such as larger magnetic moments, together with more robust remanence and longer lifetimes. A known relaxation mechanism is the vibrational coupling to substrate phonons, an effect that is a subject of study by our group. This PhD project proposal aims at constructing (and subsequently applying) effective Hamiltonians that account for phonon relaxation channels on the same footing as other essential contributions to the problem, namely intra-atomic Coulomb interactions, symmetry of the environment, hybridization with the bath and spin-orbit coupling. We will pay special attention to the 4f case, where the strongly correlated multi-orbital character is not fully captured in conventional DFT techniques. To this end, we will profit from the group's expertise in non-perturbative computational many-body techniques, which include Green's functions methods and the numerical renormalization group.

Project S5. Development of biodegradable adsorbents for the removal of emerging contaminants (pesticides, pharmaceuticals and heavy metals) from water.

Contact person: Sivina Cerveny (silvina.cerveny@ehu.eus)

Climate change and water are inseparably connected. Extreme weather events make the water on our planet scarcer, more polluted, and more erratic than ever. In addition, human activity has also resulted in increased water contamination. Over the last two decades, scientists, regulatory agencies and the European Commission have recognized that pharmaceuticals create environmental problems when these products are discharged into water. Residues of various drugs have been detected in surface water, groundwater, soil, air, and biota. Since drugs are designed to produce pharmacological effects at low concentrations, this finding has an eco-toxicological impact on microorganisms, flora, fauna, and human health. These residues have been declared "emerging contaminants". In addition to medicines, heavy metals, pesticides and other small molecules have also been detected in the water, creating a significant problem for human health and becoming a challenge for the water sector. It is important to note that existing wastewater treatment plants are not guaranteed to remove these contaminants of emerging concern.

The main objective of this PhD project is to develop innovative, efficient and profitable methods to mitigate the problem of emerging pollutants in water. The main task is to establish a fast adsorbent with the following characteristics: low cost, high efficiency in adsorbing a collection of contaminants simultaneously, and scalable to the industry. In addition, this project aims to unveil the adsorption mechanisms from a fundamental point of view. The research pursued in this proposal involves working in a multidisciplinary group where the researcher will have access to different fields of work related to medicine, nanotechnology, and water.

The student will be trained in various characterization techniques, acquiring considerable skills during this project. We seek a highly motivated PhD student with a physics, material science, or chemistry background.

Project S6. First-principles analysis of the charge-density wave transitions in Kagome topological superconductors

Contact person: Ion Errea (ion.errea@ehu.eus) and Maia G. Vergniory (maia.vergniory@cpfs.mpg.de)

The recently discovered (Cs,K,Rb)V3Sb5 metals show a plethora of correlated properties including Z2 topology, superconductivity, and electronic chiral transport [1,2,3]. All this makes them fantastic candidates for applications in novel quantum devices. The phase diagrams of these materials remain controversial as it is not clear what the origin and the ordering of the low-temperature charge-density wave (CDW) phase is and how it couples to external perturbations like strain or magnetic fields. In this project, by making use of first-principles anharmonic calculations within the stochastic self-consistent harmonic approximation (SSCHA, www.sscha.eu) developed in our group [4], we aim at understanding the CDW transitions, their origin, and how they couple with external perturbations as well as superconductivity. The candidate will learn in this project advance methods related to topology, superconductivity, anharmonicity, and electron-phonon physics, offering a broad and modern perspective of current theoretical condensed matter physics.

[1] B. R. Ortiz et al. Phys. Rev. Mater. 3, 094407 (2019).

[2] B. R. Ortiz et al. Phys. Rev. Lett. 125, 247002 (2020).

[3] C. Guo et al. Nature 611, 461 (2022).

[4] L. Monacelli et al. Journal of Physics: Condensed Matter 33, 363001 (2021)

Project S7. Moiré quantum matter in 2D-materials characterized by local spectroscopic techniques

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

Moiré super-lattices formed by stacking a couple of 2D layers are emerging as a powerful platform for studying new physical phenomena. These new phases of quantum matter hold extreme potentialities and high tunability to unlock key-technologies. The variable atomic interactions and the atomistic thickness of the materials enable to control and engineering of the electronic, magnetic, excitonic, or superconducting properties emerging at these interfaces. However, a greater knowledge of periodicity, strain, defects, and chemical and electronic doping is required.

This PhD-thesis is part of an ongoing work focusing on the formation and local characterization of opportune interfaces of 2D layers suited for strong light absorption and sensitivity, fundamental for energy conversion and photodetectors. The vapor deposition synthesis of materials in an ultra-high vacuum enables the formation of a free choice of heterostructures. Local spectroscopic techniques and the usage of a mobile sharp electrode enable their characterization and manipulation.

During this project, the student will receive training in surface science techniques and acquire various skills, such as handling ultra-high vacuum equipment, physical vapor deposition, Auger spectroscopy, and scanning probe techniques at cryogenic temperatures (liquid nitrogen and helium) for the preparation and characterization of the samples.

More information: https://cfm.ehu.es/atomic-spectroscopy/

Project S8. PhD in experimental surface electrochemistry 2D materials for water electrolysis

Contact person: Sara Barja (sara.barja@ehu.eus)

Research topics will cover the following fields: Spectroscopy, Microscopy, Instrumental development, Catalysis, Electrochemistry and Surface Science.

Development of optimized catalysts requires a comprehensive atomic scale picture of the chemical and physical properties of surfaces, in connection to their macroscopic catalytic performance. The propose research project aim at acquiring molecular level understanding of electrocatalytic processes using innovative materials tools. The range of experimental methods will comprise spectroscopic (X-Ray photoemission spectroscopy) and microscopy (scanning tunneling microscopy, atomic force microscopy) methods in both ultrahigh vacuum and ambient pressure conditions at electrochemical interfaces.

This project focuses on relevant 2D materials (graphene, MoSe2) for water electrolysis, and proposes to bridge the gap between model studies and real electrocatalytic systems. The project is embedded into interdisciplinary and international collaborations involving experimental and theory groups from materials science and electrocatalysis. The PhD-student will become party of the above project and will during his/her PhD explore complex model interfaces, covering surface science, electrocatalysis and in-situ studies. The experimental results obtained in the project aims at a mechanistic understanding of chemical processes associated with energy conversion, energy storage, chemical production and materials synthesis.

Project S9. Tuning the Assembly of Proteins in Lipid Bilayers

Contact person: Armando Maestro (armando.maestro@ehu.eus) and Ivan Sasselli (i.sasselli@csic.es)

Endocytosis, an intracellular trafficking series of processes taking place at the plasma membrane, is a striking example of how the self-assembly of membrane proteins is crucial in the different key cellular processes, such as nutrient uptake, cell signaling, etc. Besides, dysfunctional endocytic processes involving alteration in the protein assembly are linked to some types of physiopathological conditions like Alzheimer's disease, atherosclerosis, and cancer. Despite extensive molecular knowledge from structural biology and biophysics experiments, the intricate nature of endocytosis has hindered a complete understanding of this essential cellular mechanism, with critical queries regarding the role of lipids in protein assembly architecture still remaining unanswered.

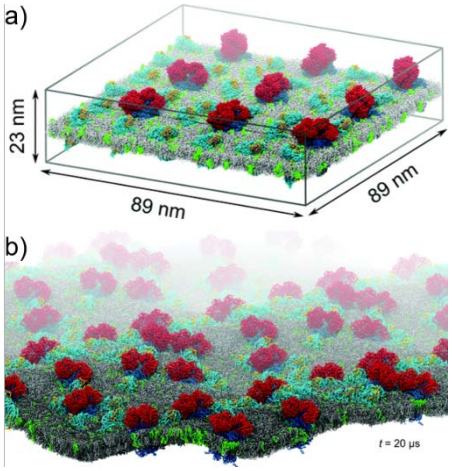

Figure 1. (a) initial set up, and (b) result after 20 µs of a protein super-complex assembly simulation in a lipid bilayer using the MARTINI model.[1]

Simultaneously with experimental research, significant progress has been made towards developing computational techniques to investigate the subject matter. These computational methods facilitate a detailed examination of the underlying interactions and present a cost-effective avenue for testing and screening new designs. The MARTINI method, in particular, has demonstrated its capacity to simulate the behaviour of protein membranes, along with their interactions and assembly.1-2 The coarse-grained nature of the model permits affordable simulation of systems at the necessary scale while preserving the required interaction resolution.

The primary objective of this PhD project is to comprehend the underlying mechanisms and driving forces that govern the formation of assemblies by the clathrin and adaptor complex

proteins,3-4 in order to manipulate the shape and features of such assemblies across various lipid membranes. By doing so, we aim to engineer proteins that assemble into novel configurations to be used not only to understand the endocytic mechanism but also to design and develop hybrid protein/lipid complexes to improve existing drug delivery systems.

The student in charge of this project will acquire knowledge on molecular dynamics (MD) simulation methods for the purpose of parameterizing and simulating target proteins, with the aim of gaining understanding on their assembly behaviour. The project will be carried out, in parallel with experiments (mainly scattering and imaging techniques) to validate the computational findings. The student can get involved in the experimental techniques to any extent that can be discussed. Ultimately, this PhD project will enable the student to integrate their computational and experimental expertise to uncover the primary interactions that dictate the assembly of the clathrin and adaptor complex proteins,3-4 leading to the development of novel and customizable membrane protein assemblies.

1. Arnarez, C.; Marrink, S.; Periole, X. Chem. Sci., 2016, 7, 4435.

2. Ingólfsson, H. I.; Arnarez, C.; Periole, X.; Marrink, S. J. J. Cell Sci., 2016, 129, 257.

3. Kelly, B. T.; Graham, S. C.; Liska, N.; Dannhauser, P. N.; Höning, S.; Ungewickell, E. J.; Owen, D. J. Science, 2014, 345, 459.

4. Doherty, G. J.; McMahon, H. T. Annu. Rev. Biochem., 2009, 78, 857.