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. Machine learning-based design of novel functional nanomaterials
Project S2. Stimuli responsive hetero-interfaces of two-dimensional materials
Project S3. Greenhouse gas sequestration at the atomic scale: Dry reforming of methane molecular beams
Project S4. Simulating cotranslational protein folding in the ribosome
Project S5. Exploring materials for quantum technologies
Project S6. Generation of 1D/2D/3D optically active nano-microstructures by femtosecond-laser-induced processing of rare earth-doped glasses: Spectroscopic characterization and performance.
Project S7. Quantum effects and optoelectronic response in plasmonic nanocavities filled with organic molecules
Project S8. Non-equilibrium dynamics of amorphous polymers and other materials
Project S9. Interaction of intelligent drug delivery vehicles with biomembranes
Project S10. Theoretical description of the infrared near-field microscopy response of hybrid polaritonic nanostructures
Project S11. Interaction of quantum light and matter at the nanometric scale for sensing and quantum computation
Project S12. Magnetism meets superconductivity

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

Due to the uncertainties regarding COVID-19, the CFM's PhD Recruitment Fair will be held, one more year, through an on-line selection process whose details will be defined during the next weeks and published in the CFM website. The process 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 16132,32 € (before taxes) during the first year, with subsequent increases of around plus 1000 euros per year, over the

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

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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 UPV/EHU before 31st December 2022 for the PhD contract to be continued. Therefore, **the candidates are required to hold a Master degree granted before the end of 2022**.

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 (follow the link above).
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 2022, 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 2022 at 13:00 CET) will be evaluated.*

LIST OF AVAILABLE PROJECTS

Project S1. Machine learning-based design of novel functional nanomaterials

Contact people: Pedro Braña (pedro.brana@ehu.eus) and Ruben D. Costa (ruben.costa@tum.de)

Are you passionate about innovation? Do you love developing applied science with real-life impact? Do you use multidisciplinary thinking to solve professional questions? Are you able to appreciate the beauty of nature's solutions to its many challenges? Would you like to innovate in an international and highly collaborative environment? Then the Theoretical and Computational Chemistry group at the CFM and the Chair of Biogenic Functional Materials at the TUM are the perfect places for your future.

Summary of the Research

We are looking for a motivated PhD student interested in machine learning. The candidate, together with a multi-disciplinary and cross-functional team, will help design, implement, and analyze machine learning and deep learning models to design novel functional nanomaterials (e.g., nanoparticles, low-dimensional materials, hybrid materials, bio-hybrids, protein-based materials, etc.) for applications in energy storage and conversion as functional materials. The validation of the design will also be carried out in the chair for biogenic functional materials at the Technical University of Munich (TUM) led by Prof. Costa. The student will participate in research programs funded by the European Commission.

Project S2. Stimuli responsive hetero-interfaces of two-dimensional materials

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

Two-dimensional materials are rising considerable attention in diverse fundamental and applied fields involving energy scavenging, photosensitivity, charge transport, magnetism or superconductivity. The still young research field and the potentialities emerging at these materials demand for new investigation of their electronic properties tuned by interface, chemical doping, defects, lattice strain and compression, etc.

This PhD thesis is part of an on-going work focusing on the characterization of the atomic structure, electronic and chemical properties occurring at these interfaces. Starting point of the investigations is the formation of metal-halides 2D-structures with strong light absorption and sensitivity, fundamental for energy conversion and photodetectors. The vapor deposition synthesis of materials in ultra-high vacuum will enable a free choice of elements for the formation of heterostructures (both organics and inorganics), control of their shape and size, doping, etc.

During this project, the student will be trained in various surface science techniques. They will acquire various skills, which include handling ultra-high vacuum equipment preparation of the

sample preparation via physical vapor deposition, sample characterization via Auger spectroscopy and state of the art scanning probe techniques at cryogenic temperatures (liquid nitrogen and liquid helium).

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

Project S3. 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 S4. Simulating cotranslational protein folding in the ribosome

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

A human cell contains over 100.000 types of unique proteins, and the information contained in its sequence of amino acids is sufficient for it to adopt its folded structure. Protein synthesis occurs on ribosomes, where the nascent chain is progressively synthesized and passes through a tunnel inside the ribosome. When the chain is formed, folding occurs and the final structure is adopted. For years this official paradigm established that the ribosomal tunnel was a passive conduct; however, today we know that protein folding begins in the ribosome tunnel itself. What happens during this transit is enigmatic since all the experimental evidence is indirect, and

poses a major theoretical-experimental challenge. It implies the experimental capacity to observe the process of creation and folding of the peptide in real time and to be able to create quantitative models through molecular dynamics in sufficiently wide time intervals.

This PhD project deals with the theoretical-computational part of an ambitious collaboration with the University of Marseille, that has the challenge of taking real-time images of the process described above, using High Speed Atomic Force Microscopy. This project aims to clarify, through theoretical simulations accompanied by HS-AFM images, the crucial role played by co-translational folding in the formation of neuronal potassium channels.

Project S5. Exploring materials for quantum technologies

Contact people: Celia Rogero (celia.rogero@ehu.eus) and Maxim Ilin (maxim.ilin@ehu.eus)

We propose a challenging experimental PhD project devoted to the development and application of materials for quantum-enabled technologies and devices. We are right now on the second quantum revolution where materials science will be key to unlocking novel technologies based on quantum properties. In this context, the aim of the PhD position will be to grow and study the properties of novel materials with potential application on quantum technologies into the future. We will mainly focus on thin film ferromagnetic insulators [1], as well as ferromagnetic semiconductor 2D Van der Waals materials [2]. This fundamental study will combine the most atomically precise growth techniques with the most sophisticated, structural, spectroscopic, magnetic characterization techniques operating under Ultra-High Vacuum (UHV) conditions, such as low temperature Scanning Tunneling Microscopy and Spectroscopy (STM, STS), or X-ray Photoemission and Magnetic Dichroism spectroscopy (XPS, XMCD).

It will be an exciting work at the interface between materials science, chemistry, condensed matter physics and quantum science. We aim to delve into the knowledge of certain **quantum technological areas**, such as, those that arise from **the coupling between a ferromagnetic insulator and a superconductor**.

We are looking for highly motivated PhD students with background in solid state physics or chemistry to work in the framework of multidisciplinary European Collaborative Projects. Daily work will be conducted at NanoPhysics Laboratory, with frequent visits to synchrotron installations as well as to CIC NanoGUNE.

References associated to this work:

[1] Nano Letters 20, 6815–6823 (2020)

[2] ACS Nano 15, 14985, (2021)

Project S6. Generation of 1D/2D/3D optically active nano-microstructures by femtosecond-laser-induced processing of rare earth-doped glasses: Spectroscopic characterization and performance.

Contact people: Rolindes Balda (rolindes.balda@ehu.eus) and Joaquín Fernández (xuaco@dipc.org)

Sequestration Research Group: **Laser Spectroscopy and Photonic Materials group,** Department of Applied Physics, Faculty of Engineering of Bilbao, University of the Basque Country (UPV-EHU).

The aim of the project is to obtain optically active vitroceramic photonic structures by laser-writing in high quality rare-earth-doped glasses for optoelectronic and biomedical applications (low coherence emitters, sensors, ...).

The study includes the characterization of the induced structural changes as well as the investigation of the optical properties of the native and laser treated samples including time-resolved spectroscopy of both bulk glass and nano-micro structures, emission efficiencies and guidance.

Project S7. Quantum effects and optoelectronic response in plasmonic nanocavities filled with organic molecules

Contact person: Rubén Esteban (ruben.esteban@ehu.eus)

The objective of this theoretical thesis is to investigate quantum effects and the optoelectronic response in state-of-the-art plasmonic nanoresonators. The interaction between organic molecules and metallic nanoresonators involves complex electronic, chemical and optical processes. The optical interaction can be strongly enhanced by the excitation of resonant collective oscillations of the free electrons of the metal, called plasmon polaritons, which can localize optical fields down to (sub)nanometric regions.

This extreme field confinement can lead to intriguing quantum effects in molecular spectroscopy. Further, for metallic nanoresonators presenting ≈1 nm thin gaps, or molecules placed very close to the metallic surface of these resonators, electron transfer processes can occur. The interplay between optical and electronic interactions in these situations often leads to a complex optoelectronic response.

The work of the student will consist in developing and applying classical and quantum methodologies, such as the cavity quantum electrodynamics framework, to investigate quantum and/or optoelectronic phenomena in these systems. A variety of topics can be explored, depending on the progress of the thesis, including non-linearities, photon correlations and optical microscopy with submolecular resolution. The work is theoretical, but collaborations with other theoretical and experimental groups are expected.

Project S8. Non-equilibrium dynamics of amorphous polymers and other materials

Contact person: Daniele Cangialosi (daniele.cangialosi@ehu.eus)

The thermodynamic state of amorphous polymers and other materials may profoundly affect their performance in a wide variety of applications, ranging from the most traditional ones to those of recent technological relevance, such as electron transport properties in materials employed for solar cells. If a system of this kind is brought to non-equilibrium conditions, its thermodynamic state may vary tremendously depending on the thermal history. This is the case of amorphous melts vitrified to their glassy state and polymers in contact to an interface, which can either adsorb or dewet.

This project aims to unveil the mechanisms behind the kinetics of evolution toward the most easily accessible stable thermodynamic state of a non-equilibrium system made of both glasses of different nature and polymers in contact with interfaces. For this purpose, calorimetric techniques, including new generation fast scanning calorimetry, will be the main methods to characterize the thermodynamic state of amorphous polymers and other materials in a wide range of conditions. Highly motivated candidates with solid background in material science and physical chemistry are sought.

Project S9. Interaction of intelligent drug delivery vehicles with biomembranes

Contact people: Armando Maestro (armando.maestro@ehu.eus) and Carlos Sánchez (carlos.sanchez@dipc.org)

Many of the therapeutic agents or modalities emerging from pharmaceutical companies, including precision cell-based therapies, rely on direct delivery into the cytosol or specific sub-cellular compartments (1,2) within the cell, for their activity. Unfortunately, many of these therapeutic strategies are impermeable to the cell membrane. Therefore, there has been a considerable interest in the development of 'intelligent' delivery systems to ensure the delivery of therapeutic agents to their intended intracellular targets.

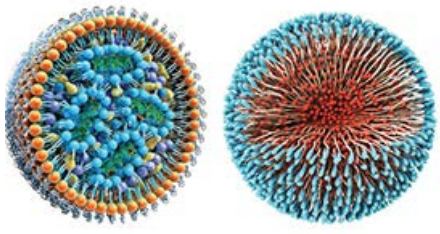

Figure 1. (Left) lipid and (Right) polymeric nanoparticles. https://drug-dev.com/nanoparticles-a-revolution-in-the-development-of-drug-delivery-vehicles/

Of particular interest in this PhD will be responsive nanoparticulate delivery systems composed of lipid, polymeric or inorganic nanoparticles (see Figure 1). The interest in those system stem from their potential to protect their payload (including RNA, proteins or other biomolecules), to increase their in vivo stability (3), to reach a specific cell or tissue, and to control the release of their cargo within desired cellular regions (2). However, despite the considerable research effort that has gone into the development of these intelligent delivery systems, the field is currently hindered by a poor understanding of how such vehicles gain access to the interior of the cell.

In this PhD proposal, therefore, different types of nanoparticles will be assembled and characterized and their interaction with biomimetic cell membranes of different complexity (including from in vitro biomimetic model systems to in vivo mammalian cells) will be studied by a combination of imaging and neutron and X-ray scattering methods.

References

(1) Stewart et al (2018) Chem. Rev. 118, 7409−7531; (2) De Geest (2018) Mol. Immunol. 98, 25−27; (3) Luo et al (2017) J. Controlled Release 263, 200−210.

Project S10. Theoretical description of the infrared near-field microscopy response of hybrid polaritonic nanostructures

Contact people: Javier Aizpurua (aizpurua@ehu.eus) and Rainer Hillenbrand (r.hillenbrand@nanogune.eu)

This thesis will focus on the theoretical analysis of infrared near-field probing (using metal tips in scattering-type scanning near-field optical microscopy, s-SNOM) of hybrid nanostructures that are composed of polaritonic nanoresonators (e.g. made of polar materials such as hBN hosting phonon polaritons) and molecules possessing infrared vibrational response. When the nanoresonator efficiently couples with molecular layers showing vibrational fingerprints at infrared energies, the electromagnetic near-field response of the hybrid system is challenging to interpret.

While some studies have addressed the near-field response of such complex systems via simple models that do not consider the realistic geometry and detection schemes (tip modulation and signal demodulation), much work remains ahead to understand the near-field response encoded in the measured s-SNOM signals.

This thesis will study the effect of the probing tip on the properties of the near-field in phononic resonators coupled to molecular layers. Realistic tips, as well as the effect of demodulation will be theoretically tackled directly under the supervision of the “Theory of Nanophotonics” group at MPC, in selected nanomaterials relevant to experimental implementations of phononic resonators as developed at the “Nanooptics Laboratory” at nanoGUNE. A variety of classical electrodynamics tools will be mastered in the development of this thesis.

Project S11. Interaction of quantum light and matter at the nanometric scale for sensing and quantum computation

Contact people: Gabriel Molina-Terriza (gabriel.molina@ehu.es) and Miguel Varga (miguel.varga@ehu.eus)

The advent of exotic sources of light which can only be described using quantum mechanics, has allowed to investigate new regimes of light-matter interaction. This has found new applications

in metrology as certain measurements can achieve high sensitivity in these regimes. Among other applications, quantum light scattering with nanostructures is a powerful method for measuring material characteristics without destroying the sample. In the field of quantum computation, this interaction can be understood as a logical gate in order to build the first steps of a quantum computer.

In this project, the student will develop a system for doing scattering of entangled photons off nanometric structures and also its propagation through multimode fibers.

The student will work with a photon source already mounted and learn how to modify their spatial and spin structure. After controlling the photon source, they will make the photons interact with structures located inside an optical cryostat. In addition to the experimental work, the student will develop the theoretical frame for understanding and analyzing the obtained results. The student will be supported by the Quantum Nanophotonics Laboratory team, in a friendly, engaging and inspiring environment.

Project S12. Magnetism meets superconductivity

Contact people: 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.

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