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. Theoretical Modelling and Experimental Realization of Proteins as Active Energy Conversion Materials
Project S2. Molecular Dynamics Study of Calmodulin in Potassium Channels
Project S3. Phase Behavior and Metastability in Hybrid Perovskites for Photovoltaic and Photonic Applications
Project S4. Effect of Secondary Interactions on The Structure and Dynamics of Soft Matter
Project S5. Stabilized Single-Chain Nanoparticles (SCNPs) for Advanced Applications
Project S6. Dynamics and Kinetics of the CO-O Recombination at Surfaces Studied from First-Principles Based on Machine Learning Potentials and Transition State Theory
Project S7. Structure and Dynamics of Complex Polymer-based Materials for Energy Storage: Insights from Neutron Scattering and Other Complementary Experimental Methods
Project S8. Synthesis of Functional Materials for Chemical Synthesis
Project S9. On the Quest for New Magnetic 2D Materials
Project S10. Functional Metal-Organic Platforms for Energy Conversion or Storage
Project S11. Magnetism Meets Superconductivity
Project S12. Light-Controlled Quantum Dots-Based Plexcitonic Emitters for Quantum Technology Applications
Project S13. Non-Equilibrium Dynamics of Amorphous Polymers and Other Materials
Project S14. Synthesis and Electronic Structure of One-Atom-Thick Hexagonal Boron Nitride on Curved Crystals: Toward Boron Nitride Nanostripes
Project S15. Development of Eco-Friendly Membranes for Water Remediation and Packaging
Project S16. Unveiling the Structure-Activity Relationships for Water Electrolysis
Project S17. Spin-Dependent Transport Properties of Non-Conventional Superconductors with Magnetic Impurities
Project S18. Hybrid Plasmonic Nanostructures for Neuronal Photostimulation
Project S19. Thermodielectric Properties of Nano-Porous Aluminosilicates
Project S20. Computational Design of Self-Healing Materials Made of Topologically Complex Polymers
Project S21. Coupled Vibrational and Electronic Spin Systems
Project S22. Exploring Materials for Quantum Technologies

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

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

7 PhD studentships available

Due to the situation with the COVID-19 pandemic, it was necessary to cancel the on-site part of CFM's PhD Recruitment Fair. It will be replaced by 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, seven (7) candidates will be selected and granted full studentships. Each studentship will cover a period of three years, including a salary of 16.131,72 € (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 UPV/EHU before 31st December 2021 for the PhD contract to be continued. Therefore, **the candidates are required to hold a Master degree granted before the end of 2021**.

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 20th April 2021, 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.

[2] *Only applications received before the deadline (20th April 2021 at 13:00 CET) will be evaluated.*

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Final Selection Process: Soon after the on-line interviews, the committee will select the 7-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

LIST OF AVAILABLE PROJECTS

Project S1. Theoretical Modelling and Experimental Realization of Proteins as Active Energy Conversion Materials

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

We have recently shown that fluorescent proteins (FPs) can be stabilized in a polymer matrix that keeps their functionality long enough to allow their application in optoelectronic applications. However, there is an issue that must be solved for their real-life application, namely, understanding the nature of the protein-polymer matrix interaction to maximize stability.

The Ph.D. candidate will use theoretical models and hybrid quantum mechanics/molecular mechanics/molecular dynamics (QM/MM/MD) simulations to unravel the stabilization mechanism of proteins in polymer matrices. In a second step, this information will be used to design a new photomultiplier coating based on singlet fission to realize a new generation of single-layer silicon solar cells bypassing the Shockley-Queisser limit. Specifically, FPs will be modified to incorporate a suitable singlet fission (SF)-active chromophore and a red-emitting molecule to enable down-conversion of energy and energy transfer (ET) to silicon.

The candidate will use QM/MM methods and model Hamiltonian approaches to simulate the dynamics of SF and ET of models of the systems investigated to find the optimal combination that maximizes the yield of the overall energy conversion process. This will pave the way for the experimental realization of the device in collaboration with the experimental group of Prof. Costa.

Project S2. Molecular Dynamics Study of Calmodulin in Potassium Channels

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

The complete resolution of the sequence of the human genome in 2016 has been a huge milestone that continuously reveals causal relations among pathologies and gene signaling. Moreover, the latest advances of experimental techniques, such as nuclear magnetic resonance, provide a direct access to 3D maps with atomic resolution of the proteins that form cell

membranes. This new accessible structural information has become a revolution in biological sciences for the design of new drugs that improve the well-being of humans. Remarkably, 60% of the commercial drugs act precisely on the proteins located at the cell membranes.

With this scenario in mind, physical models that mimic atomic interactions within the proteins and their posterior time evolution through molecular dynamics provide a very powerful tool for the prediction and comprehension of membrane phenomena. Theoretical simulations of proteins serve as guidance for the design of new drugs and help understanding the enormous amount of experimental information available.

In this project we shall consider the Kv7.2 channel of neuron membranes — a potassium voltage-gated channel located in human neurons —whose functioning relies on a potential difference induced by calmodulin (CaM). By means of all-atom simulations, molecular dynamics and coarse grain models, we would like to validate two claims regarding the behavior of the secondary structure of the IQ motiv of the channel:

1) Both wild type and mutant can form stable helices without the ribosome;
2) Wild type can form an alpha helix at the ribosome whereas the mutant cannot.

Candidates must hold a degree in physics or chemistry, with a solid background in programming. Knowledge on molecular dynamics will also be valuable.

Project S3. Phase Behavior and Metastability in Hybrid Perovskites for Photovoltaic and Photonic Applications

Contact people: Felix Fernández-Alonso (felix.fernandez@ehu.eus) and Kacper Drużbicki (kacper.druzbicki@ehu.eus)

The PhD candidate will join the *Quantum Beams & Sustainable Materials Group* at the Materials Physics Center. The group primarily uses neutron and X-ray scattering techniques in combination with atomistic modelling to interrogate and understand novel functional media for energy applications and sustainability, in close collaboration with leading international laboratories from around the globe.

The primary aim of this project is to explore the properties and phase behavior of hybrid perovskites using these methodologies. In particular, this project is part of wider efforts to understand and ultimately tailor the regimes of stability and metastability of this emerging family of materials as a function of external parameters such as temperature, pressure or chemical environment, as well as to unveil the mechanisms underpinning photovoltaic performance and degradation pathways under physico-chemical conditions of technological relevance. We anticipate that this body of work will pave the way for new and much-needed insights into the primary bottlenecks currently hampering the widespread use of hybrid perovskites in photovoltaic and photonic applications.

Project S4. Effect of Secondary Interactions on The Structure and Dynamics of Soft Matter

Contact people: Ángel Alegría (angel.alegria@ehu.eus) and Silvia Arrese-Igor (silvia.arreseigor@ehu.eus)

The dynamics and basic physical properties of soft matter are governed by their molecular structure. In addition to the covalent bonds defining the chemical structure of organic materials, the presence of secondary interactions such as hydrogen or ionic bonds can favor the formation of supramolecular mesostructures. Due to the non-permanent nature of the mentioned bonds, resulting structures can range from stable to unstable depending on several external physical parameters. A current challenge in the field is to gain deeper insight into the microscopic dynamics of such systems, its relation to the dynamic equilibrium of the formed structures and their impact on their basic physical properties, including the effect of secondary interactions on fundamental physical phenomena like the glass transition, aging, or the rheology of glass forming systems.

In the pursuit of these goals, the PhD project will consist on the study of the supramolecular structure and dynamics of systems showing secondary (non-covalent) intermolecular interactions/bonds from a fundamental point of view. The problem will be approached by combining multiple experimental techniques available in the Polymers and Soft Matter Group laboratories including but not limited to; Broad Band Dielectric Spectroscopy, Shear dynamic test, Differential Scanning Calorimetry, and Small Angle X-ray Scattering.

Project S5. Stabilized Single-Chain Nanoparticles (SCNPs) for Advanced Applications

Contact person: Josetxo Pomposo (josetxo.pomposo@ehu.eus)

Trying to mimic the outstanding functionalities of enzymes and intrinsically disordered proteins (IDPs) the research field of folding functionalized synthetic polymers to single-chain nanoparticles (SCNPs) has flourished in recent years. The folded conformations of SCNPs produce robust SCNPs when stabilized by covalent interactions. Conversely, when folding results from noncovalent interactions such as hydrogen bonds, host-guest interactions, metal complexation, p-p stacking and hydrophobic interactions, dynamic SCNPs are obtained. Even if current single-chain technology still lacks the nature´s exquisite degree of control to generate 3D-proteins, some SCNPs already mimic the outstanding properties of antimicrobial polypeptides, as well as both the size and function of structural proteins, IDPs and metallo-enzymes. The present project aims to produce stabilized SCNPs -free from aggregation issues often observed in highly concentrated solutions of SCNPs- paving the way to advanced applications of these soft nano-objects in all-polymer nanocomposites, tunable catalytic nanoreactors, crowding-sensitive probes, and so on. An in-depth characterization of these synthetic nano-objects will be also carried out.

We are looking for a motivated candidate with a degree in Chemistry, Physics or related field, Master degree, very good academic record, very good level of English, and hands-on experience (or familiarity) on synthetic procedures and on standard characterization techniques.

Project S6. Dynamics and Kinetics of the CO-O Recombination at Surfaces Studied from First-Principles Based on Machine Learning Potentials and Transition State Theory

Contact person: Joseba Iñaki Juaristi (josebainaki.juaristi@ehu.eus)

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 pre-adsorbed CO. There are experiments showing that the efficiency of these processes depend dramatically on the metal surface considered and on coverage. The objective will be to determine the surface electronic properties that cause such dependence. To this aim, machine learning potentials based on ab-initio electronic structure calculations will be generated that will allow to perform high dimensional molecular dynamics simulations for several coverages and surfaces of interest. Furthermore, molecular dynamics together with transition state theory will be applied to calculate the rate constants for the relevant competitive reactions.

The PhD candidate will acquire a strong background in theoretical chemical physics, including density functional theory, electronic structure calculations, molecular dynamics methods, transition state theory, scientific programming, and machine learning techniques.

Project S7. Structure and Dynamics of Complex Polymer-based Materials for Energy Storage: Insights from Neutron Scattering and Other Complementary Experimental Methods

Contact people: Arantxa Arbe (a.arbe@ehu.eus) and Jon Maiz (jon.maizs@ehu.eus)

Ferroelectric polymers are gaining importance for data storage methods in which bits are recorded based on the polarization directions of individual domains. These materials present an intrinsic bistable, remnant polarization whose direction can repeatedly be switched by an electric field. Films of polymer blends are promising for their ferroelectric properties and application as energy storage medium.

This project focusses on complex polymer-based materials where polymer chains are mixed with other entities, leading to polymer blends or nanocomposites. The impact of internal structure and topology of the incorporated structural units (e.g. linear chains and/or Single Chain

Nanoparticles) on the structure and dynamics of such compounds will be investigated. One of the major challenges is the component-selective characterization of the obtained material at microscopic level. In this context, scattering techniques and, particularly, neutron scattering, are especially appropriate. Neutron scattering carried out at large facilities encompasses a set of non-destructive experimental techniques that enable the selective and molecular analysis of complex systems over a broad range of length and time scales. Complementary techniques (calorimetry, rheology, dielectric spectroscopy, Small and Wide Angle X-ray Scattering) available in our labs are also essential to complement these studies, addressing the processing-structure-function relationships of such systems.

Project S8. Synthesis of Functional Materials for Chemical Synthesis

Contact people: Martina Corso (martina.corso@ehu.eus) and Dimas G. de Oteyza (d_g_oteyza@ehu.eus)

We are looking for highly motivated candidates, physicists or chemists, with a background in solid state physics, surface science or physical chemistry to take up an experimental PhD position in the area of functional carbon-based nanomaterials.

In this challenging PhD project, several strategies will be explored to create atomically precise carbon-based nanostructures with specific functionalities to detect toxic gases and air contaminants. The ultimate goal is to create materials with enhanced sensitivity and selectivity to specific analytes. The specific functionalities in the graphenic nanoscale materials, as graphene nanoribbons, will be included in the materials during their growth by means of on-surface synthesis in ultra-high vacuum conditions. The electronic response to different analytes of the functionalized materials will be tested with surface sensitive characterization tools such as scanning tunneling microscopy/spectroscopy (STM/STS), X-ray photoelectron spectroscopy (XPS) and Angle-resolved photoemission (ARPES).

The successful candidate will be integrated in a multidisciplinary national collaborative project and in the international working environment of the NanoPhysics Laboratory.

Project S9. On the Quest for New Magnetic 2D Materials

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

Our research today focuses on magnetic properties of 2D materials which are induced either extrinsically by depositing adatoms and magnetic clusters, such as those composed of transition metals and their oxides, or intrinsically by being built themselves from transition metal oxides. Our research does not exclude possible studies to made some studies into the world of Heusler alloys, considered some of them to be today topological insulators, going beyond the well-known expertise in the group on Heusler shape memory alloys.

The interest of this research comes in view of the role played by localized electronic states in electron properties related to magnetism and superconductivity and measured already in several experiments on 2D materials.

PhD candidates are required to have studied Physics or related fields that show previous experience on density functional theory (DFT) functional methods such as VASP…. Previous theoretical knowledge during the master in subjects such as magnetism, Heusler alloys and nanostructures would be highly valuable.

Project S10. Functional Metal-Organic Platforms for Energy Conversion or Storage

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

The careful and free selection of the constituents has made organic/inorganic hybrid structures one of the most interesting and versatile platforms for different areas of fundamental and applied research. Yet, any improvements in material efficiency and suitability for applications, for example for energy conversion or storage, still proceed by trial and error. Thus, the fastest way to achieve functional devices requires a better understanding of fundamental aspects as charge-transport and chemical stability of the structures in working conditions.

The present project focuses on the evaluation of the structural and electronic response of these hybrid interfaces under external driving as temperature, electric-field, light and coadsorbates. This response will be characterized by local measurements of nano-structures of 0 to 2-dimensions supported on surfaces. By visualizing the electronic and structural properties with atomic spatial resolution in real space using scanning probe techniques (STM, STS, AFM) in ultra-high-vacuum and at 1-Kelvin, we clarify the fundamental physical/chemical processes occurring under applied stimuli and their energy conversion/storage capability.

The candidate will acquire additional skills, as handling ultra-high-vacuum techniques and sample preparation, dealing with cryogenic temperatures (liquid nitrogen/helium), state of the art scanning-probe techniques, physical-chemical approaches of surface science.

Further information at https://cfm.ehu.es/atomic-spectroscopy/

Project S11. Magnetism Meets Superconductivity

Contact people: Nicolás Lorente (nicolas.lorente@ehu.eus) and Deung-Jang Choi (deungjang.choi@ehu.eus)

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 states. 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.

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 S12. Light-Controlled Quantum Dots-Based Plexcitonic Emitters for Quantum Technology Applications

Contact person: Yury Rakovich (yury.rakovich@ehu.eus)

The research field of quantum technologies offers significant opportunities in quantum key distribution, quantum simulation and computation, metrology, and imaging. These applications require the use of quantum emitters that can generate single photons or pairs of entangled photon pairs on demand. Luminescent quantum dots, can produce a highly coherent single-photon emission, are very promising as emitters with high single-photon purity, indistinguishability, and brightness, with extra functionality to generate photon pairs, resulting from biexciton recombination. Nanoscale plasmon–exciton (plexciton) interaction can significantly improve the emission properties of quantum dots due to the appearance of hybrid plexciton states serving as even more advanced quantum emitters. The main goal of the present project is to design and implement highly efficient plexcitonic quantum emitters operating as on-demand sources of pure single indistinguishable photons and pairs of entangled photons using theoretical, machine learning and experimental techniques.

The candidate is expected to have Master in Materials Science, Nanoscience or Photonics. Previous experience is preferred in one or more of the following areas: plasmonics, optics, luminescent nanocrystals, quantum dots, optical spectroscopy. Good written and oral communication skills in English are required.

Project S13. 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 its performance in a wide variety of applications. 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 of 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 S14. Synthesis and Electronic Structure of One-Atom-Thick Hexagonal Boron Nitride on Curved Crystals: Toward Boron Nitride Nanostripes

Contact person: Frederick Schiller (frederikmichael.schiller@ehu.eus)

Two-dimensional and one-dimensional materials are attracting strong interest due to their promising electronic, magnetic, or mechanical properties. Among them the heavily investigated graphene, a material that was once supposed to replace silicon in device fabrication. Graphene devices have been realized in certain applications (Sensoring, Biomedicine), but it cannot be used in electronics because it lacks a semiconducting band gap. Hexagonal boron nitride (hBN) is the isostructural semiconducting counterpart of graphene, and hence of fundamental importance in the development of nanolectronics applications. Yet the synthesis and electronic characterization of 2D hBN monolayers and 1D nanostructures, such as nanostripes, is poorly developed, requiring intensive search of appropriate growth substrates and fine characterization using surface science techniques.

We have recently demonstrated that hBN and graphene can be grown on curved Ni and Rh crystals, leading to homogenous coating and one-dimensional nanostripe arrangement [1]. The candidate will focus on the exploration of the structure and the electronic properties of pure and mixed hBN and graphene nanostructures on nanopatterned substrates, using Scanning Tunneling Microscopy, Low-Energy Electron-Diffraction, X-ray and Angle-Resolved Photoemission in our laboratory, as well as X-ray absorption and core-level photoemission in European Synchrotron radiation facilities.

[1] L. Fernandez et al, 2D Mater. 6 (2019) 2025013; arXiv: http://arxiv.org/abs/1811.09291

Project S15. Development of Eco-Friendly Membranes for Water Remediation and Packaging

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

The presence of metals, pharmaceuticals and other contaminants in freshwater is considered a global threat that demands effective and affordable solutions. Once water is contaminated, it is difficult, costly, and often impossible to remove the pollutants. Still today, 80 per cent of global wastewater goes untreated, containing everything from human waste to highly toxic industrial discharges. The nature and amount of pollutants in freshwater determines the suitability of water for many human uses such as drinking, bathing, and agriculture.

In this thesis, we will implement a new approach to remove pharmaceuticals of polluted waters based on the development of low-cost multifunctional nanostructured membranes to produce safe drinking water for people, irrigation and livestock. We will use different types of biopolymers and biodegradable nanoparticles. The development of these membranes requires overcome scientific and technological challenges such as the understanding of the interaction between biopolymers, nanoparticles and drugs; the functionalization of the nanoparticles and the relationship between nano- and macro-scale properties.

The project is multi-disciplinary and it involves a variety of experimental techniques available in the polymers and soft matter group (Differential Scanning Calorimetry, Broadband Dielectric Spectroscopy, AFM, TEM/SEM, etc.). In addition, these advanced characterization techniques will also allow studying the fundamentals of hydration in biopolymers.

The candidates should have a Master in Physics, Chemistry, Materials Science or Nanoscience. Previous experience in biodegradable polymers, polymer physics as well as in nanostructured materials is welcome. Good written and oral communication skills in English are required.

Project S16. Unveiling the Structure-Activity Relationships for Water Electrolysis

Contact people: Sara Barja (sara.barja@ehu.eus) and Enrique Ortega (enrique.ortega@ehu.eus)

Development of optimized catalyst requires a comprehensive atomic scale picture of the chemical and physical properties of surfaces, in connection to their macroscopic catalytic performance. Operando imaging and spectroscopy has become a cornerstone in the development of novel catalyst systems.

We combine ultra-high-vacuum characterization (scanning tunnelling microscopy, X-Ray photoemission spectroscopy), and parallel electrochemical test on the very same sample. The described experimental approach allows unique quasi-in situ studies to understand the electrode-electrolyte interface at the atomic-scale.

This project focuses on relevant metal-oxide surfaces for water electrolysis, and proposes to bridge the gap between model studies and real electrocatalytic systems. The PhD-student will become party of the above project and will during his/her PhD obtain extended experience in surface science and fundamentals of catalysis.

The experimental results obtained in the project together with theoretical models and materials synthesis will form a circular development loop aimed at optimizing catalyst performance. The multidisciplinary character of project will support active collaboration with worldwide research groups in surface science and catalysis. Such comprehensive characterization will provide the fundamental understanding of the structure-functionality relationships needed to develop new and improved electrocatalyst for clean water electrolysis.

Project S17. Spin-Dependent Transport Properties of Non-Conventional Superconductors with Magnetic Impurities

Contact people: Sebastián Bergeret (fs.bergeret@csic.es) and José Ignacio Pascual (ji.pascual@nanogune.eu)

The presence spin-orbit interaction (SOI) breaks spin degeneracies of electronics bands in materials. In superconductors, SOI may lead to non-conventional pairing schemes, with potential application in quantum spintronics.

This PhD project combines experimental and theoretical methods to study spin-resolved spectral and transport properties of superconductors with a non-conventional order parameter in the presence of magnetic impurities.

The student will first develop a theoretical framework to study spin-dependent transport, utilizing theoretical techniques for the study of electronic transport, such as Keldysh formalism, Green's functions and effective actions. In a second phase, the student will perform atomically precise tunneling spectroscopy measurements of spin-dependent transport through isolated magnetic atoms and molecules on superconductors with strong SOI. The measurements will be performed at the low-temperature STM facilities in CIC Nanogune, where she or he will also acquire training in experimental techniques. The PhD student will apply the theoretical models to interpret the spectroscopy measurements and identify the presence of spin-polarized superconductor states and their role in spin-transport.

A highly motivated student with a solid background in quantum transport, condensed matter physics, both from a theoretical and experimental perspective is sought for the project.

Project S18. Hybrid Plasmonic Nanostructures for Neuronal Photostimulation

Contact person: Marek Grzelczak (marek.grzelczak@dipc.org)

The use of light to control neuronal activity has become an emerging field of research that can enable new technologies for monitoring brain activity and establish new therapeutic means. One of the promising yet highly unexplored nanomaterials for neuronal photoactivation are plasmonic nanoparticles. By converting light into heat, plasmonic nanoparticles can stimulate neurons directly by activating thermosensitive channels without using actuators or genetic modifications.

This project aims to design and develop bio-compatible plasmonic heterostructures with optimised photothermal properties for later use in optical manipulation of neuronal activity. The selected student will have an opportunity to work in a highly interdisciplinary environment comprising nanochemistry and computational plasmonics at research centres in the San Sebastian area as well as biology and neuroscience through an internship at the Neurotechnology Center at Columbia University (USA).

The candidate is expected to have a Master in Chemistry, Materials Science or Nanoscience. Previous experience is preferred in one or more of the following areas: colloid chemistry, plasmonics, optical spectroscopy or nanomedicine. Good written and oral communication skills in English are required.

Project S19. Thermodielectric Properties of Nano-Porous Aluminosilicates

Contact person: Jorge Sánchez - Dolado (jorge_dolado002@ehu.eus)

We are looking for highly motivated PhD students with background in Physics, Chemistry, Engineering or generally Material Science to work under the umbrella of two multidisciplinary European Projects.

The project aims at exploring the impact of the nanoporous topology on several engineering properties of crystalline and amorphous aluminosilicates (zeolites, clays and cement-based materials). In particular, two main aspects will be studied:

On the one hand, the possibility of tuning the porosity for controlling the effective transport properties of these materials. Parameters like the guest diffusivities, thermal and electrical conductivities will be investigated and placed in the context of CO2 trapping and thermal and electrochemical energy storage applications [1, 2].

On the other hand, the possibility of tuning the nano-porosity for controlling the effective dielectric response of the materials. With the aim of designing new Radiative Cooling Materials [3, 4], the nano-porosity will be tuned to enhance the reflectance of solar radiation and focus the radiative emissivity within the so-called Atmospheric Window.

Depending on the candidate profile and his/her interest, the PhD project can be either experimental or theoretical.

[1] Sato, K., Hunger, M. Carbon dioxide adsorption in open nanospaces formed by overlap of saponite clay nanosheets. *Commun Chem* 3, 91 (2020). https://doi.org/10.1038/s42004-020-00346-5

[2] https://nrg-storage.eu

[3] Nature 577, 18-20 (2020), doi: https://doi.org/10.1038/d41586-019-03911-8

[4] https://cfm.ehu.es/cfm_news/the-science-of-concrete-that-could-work-the-miracle

Project S20. Computational Design of Self-Healing Materials Made of Topologically Complex Polymers

Contact person: Ángel Moreno (angeljose.moreno@ehu.eus)

Polymer-based materials with self-healing properties can be designed by implementing reversible bonds (metal-ligand, dynamically covalent, etc) in the polymer architecture, which can form intra- and intermolecular reversible cross-links, and allow for exploiting the adaptability of the topology of the dynamic bond network to strains, shear flow or other changes of the environment (temperature, pH, light, etc). The use of functionalized fully polymeric nanoparticles (nanogel-like, stars, rings, etc) as the building blocks is a promising route for the design of smart materials that combine self-healing properties with specific functions (encapsulation, catalysis, luminescence, etc). Key factors that ultimately control the stability and the mechanical and dynamical properties of the material are the specific topology of the nanoparticle and the competition between reversible intra- and inter-molecular bonding.

The aim of this PhD project is to systematically investigate in "silico", by means of large-scale molecular dynamics simulations, the role of these factors on the formation and properties of reversible self-healing materials based on such polymers. We look for a young candidate interested in theory/simulation and in soft matter physics. Background in both them will be highly esteemed.

Project S21. Coupled Vibrational and Electronic Spin Systems

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The main objective of this project is to understand the coupling between atomic vibrations and electronic degrees of freedom in systems with sizeable spin-orbit coupling. This latter introduces a real space modulation of the system phonon modes, even in the absence of a net magnetization and requires to account for the magnetic component of the induced potential. In a metal, one can imagine the hotspots of the electron-phonon matrix elements at the Fermi surface to be modulated or displaced, as the magnetic components of the potential act effectively as a real space rotation operator in spin ½ space. In particular, we will study the impact of the magnetic component of phonons in electronic transport and the spin relaxation of different magnetic adatoms on surfaces.

The project combines the use of new methodology with modelling using state of the art theoretical treatments. It includes the participation in the improvement of already developed computational tools, the development of additional modelling, focusing on the tensorial character of the spin orbit coupling, and the application to particular problems for which experimental data are available. The candidate should have a good background in solid state and many-body physics, as well as some experience in computation.

Project S22. Exploring Materials for Quantum Technologies

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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. The novel materials will cover from thin layers of inorganic materials [1, 2], monolayers of 2D Van der Waals materials [3] and organic materials [4].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 are looking for highly motivated PhD students with background in solid state physics or chemistry to work in the framework of a multidisciplinary European Collaborative Projects. Daily work will be conducted at NanoPhysics Laboratory, with frequent visits to synchrotron installations as well as to Nanogune.

[1] Nano Letters 20, 6815-6823 (2020)

[2] arXiv:2012. 15549

[3] J. Phys. Chem. C 2019, 123, 45, 27802-27810

[4] Nature 583, 48-54 (2020)