31.03.2020 COVID-19 Update:
Due to the exceptional situation with the COVID-19, some aspects of the selection process had to be modified.

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. Advanced Nanostructured Materials for Artificial Photosynthesis

Project S2. Exploiting Atomistic Molecular Dynamics Simulations to Unravel Structural and Dynamic Properties in Different Aqueous Systems

Project S3. Development and Applications of the Stochastic Self-consistent Harmonic Approximation

Project S4. Synthesis and Electronic Structure of One-Atom-Thick Hexagonal Boron Nitride on Curved Crystals: Toward Boron Nitride Nanostripes

Project S5. Generation of 1D/2D/3D Optically Active Nano-Microstructures by Femtosecond-Laser-Induced Processing of Rare Earth-Doped Glasses: Spectroscopic Characterization and Performance

Project S6. Topological and Electronic Properties of Two-dimensional Materials: Van der Waals Graphene and 2D Metal Chalcogenides Nanostructures

Project S7. Molecular Dynamics of Supramolecular Systems

Project S8. Energy Storage Solutions based on Zeolite-based Templates and Supercritical Fluids (SCF)

Project S9. Next-Generation Single-Chain Nanoparticles (SCNPs) Endowed with Multiple Functions

Project S10. Non-Equilibrium Effects in Superconducting Hybrid Structures with Spin-Orbit Coupling

Project S11. Non-Equilibrium Dynamics of Amorphous Polymers and Other Materials

Project S12. Surveying Chemical Reactions at Surfaces and Interfaces Properties

Project S13. Bringing Functional Molecular Systems onto Non-Metallic Surfaces

Project S14. Novel Carbon-Based Nanofluids for Energy Storage

Project S15. Quantum Effects in Atomic-Scale Nanophotonics

Project S16. Machine Learning for Understanding Structure and Dynamics of Polymers and Biopolymers

Project S17. Exploring Superconductor/Ferromagnetic Interfaces in Quantum Applications

Project S18. Understanding Catalytic Reactions In-Operando at the Atomic Scale: Curved Surfaces at Ambient Pressure

Project S19. Fundamental Properties of Magnetic Topological Insulators and their Heterostructures

Project S20. In Silico Design of Self-Healing Materials Made of Polymeric Nanoparticles

Project S21. Quantum Sensing based on Levitated

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

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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 2020 for the PhD contract to be continued. Therefore, **the candidates are required to hold a Master degree granted before the end of 2020**.

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 has been extended until 20th April 2020, at 13:00 Central European Time (CET)[2].

Pre-Selection Process: The applications will be evaluated by an academic Evaluation Committee at CFM. It will be composed of four (4) permanent members of the CFM faculty (Aitor Bergara, Silvina Cerveny, Iñaki Juaristi and Nerea Zabala), who will consider the CVs of the candidates, their background adequacy to the selected projects and the provided reference letters.

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[2] *Only applications received before the extended deadline (20th April 2020 at 13:00 CET) will be evaluated.*

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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 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. Advanced nanostructured materials for artificial photosynthesis

Contact person: Yury Rakovich (yury.rakovich@ehu.es) and Marek Grzelczak (marek.grzelczak@dipc.org)

The control over the materials structure down to nanoscale as well as their electronic structure are essential requisites for developing artificial photosynthetic systems that through photocatalytic conversion can efficiently store light energy in chemical bonds. Especially noteworthy is the nanomaterials composition that defines the light-harvesting capacity and drives catalytic reactions via electron transfer. The aim of this project is the rational design and development of hybrid nanoparticle-based photocatalytic systems for improved environmental remediation, using a variety of sub-units such as molecules, supramolecular complexes, plasmonic nanoparticles and quantum dots to be later assessed on a single particle level. The project is multi-disciplinary and involves a variety of techniques, ranging from fabrication of nanostructures to their characterization using absorption, photoluminescence and Raman spectroscopy, fluorescence confocal lifetime microscopy as well as fluorescence correlation spectroscopy and dynamic light scattering. The material development and advanced characterization techniques will serve to study the fundamentals of photocatalytic processes related to artificial photosynthesis with particular focus on cofactor regeneration.

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

Project S2. Exploiting Atomistic Molecular Dynamics Simulations to Unravel Structural and Dynamic Properties in Different Aqueous Systems

Contact person: Fernándo Álvarez (fernando.alvarez@ehu.es) and Juan Colmenero (juan.colmenero@ehu.eus)

In the group of 'Polymers & Soft Matter' of the Materials Physics Center, we are currently carrying out a strong effort to contribute to shed some light in the cumbersome problem of understanding the behavior of water in different environments, something which is of utmost importance, not only on biological grounds, but also from the point of view of basic science. Despite the miscellaneous existing force fields to perform atomistic molecular dynamics simulations of water, and the overwhelming experimental results on different aqueous systems and environments, a full understanding of the structure and dynamics of such systems is still lacking. Concerning atomistic simulations, one of the main problems is that standard force fields habitually used poorly reproduce one of the most relevant properties of water: the dielectric relaxation behavior. The work proposed in this project deals with (i) the modification of existing force fields to be validated not only with neutron scattering but also with dielectric spectroscopy results; (ii) the application of such force fields to simulate water in different aqueous systems; and (iii) using these simulations, -together with experimental results- to unravel structure and dynamic properties of water in such systems.

Project S3. Development and applications of the stochastic self-consistent harmonic approximation

Contact person: Ion Errea (ion.errea@ehu.eus)

The goal of this PhD project is to contribute to the development of the stochastic self-consistent harmonic approximation (SSCHA) code and use the new implementations to solve physical problems of current interest.

The SSCHA is a method that allows to calculate vibrational properties of solids including quantum and anharmonic effects in a non-perturbative way. It also allows to relax crystal structures using an energy landscape that fully includes the quantum fluctuations of the atoms. This kind of calculations are crucial to understand and predict high-temperature superconducting hydrides [1, 2], charge-density wave (CDW) materials [3], thermoelectric materials [4], and many other materials close to phase transitions.

The candidate will work on the implementation of a new way of imposing the symmetries to the SSCHA code, which will make the code much more efficient, and will work on applications especially in superconducting hydrides and CDW systems.

Project S4. 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.

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

Project S5. Generation of 1D/2D/3D optically active nano-microstructures by femtosecond-laser-induced processing of rare earth-doped glasses: spectroscopic characterization and performance

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

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 S6. Topological and Electronic Properties of Two-dimensional Materials: Van der Waals Graphene and 2D Metal Chalcogenides Nanostructures

Contact person: Andrés Ayuela (andres.ayuela@ehu.eus)

Within condensed matter, we aim to study the electronic and topological properties of graphene heterostructures, such as bilayers and bilayer flakes, with other 2D materials. We will study topological states in carbon-based nanostructures and other 2D materials, including grain boundaries and deformations. We will furthermore look at the interplay between localized states of different origins: related to edges (vacancies, ad-atoms or defects) and topologically protected states. This work will be mainly performed using methods within density functional theory, and tight binding methods implemented in the group.

Project S7. Molecular dynamics of supramolecular systems

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

The dynamics and basic physical properties of numerous liquids and solids are governed by their molecular structure. In addition to the covalent bonds defining the chemical structure, the presence of secondary interactions such as hydrogen bonds can favor the formation of supramolecular structures. Due to the non-permanent nature of the mentioned interactions, resulting supramolecular structures can range from stable to unstable depending on several external physical parameters. A current challenge is to gain deeper insights 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. With the aim of linking structure to properties from a fundamental point of view, the PhD project will consist on the study of the structure and dynamics of systems showing supramolecular arrangements. 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 S8. Energy Storage solutions based on zeolite-based templates and Supercritical Fluids (SCF)

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

The proposed project aims at exploring a set of new ideas with high theoretical and practical potential in the field of energy storage that aim to provide affordable-cost solutions in a large

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spectrum of applications (e.g. thermal power plants, concentrating solar power, compressed air energy storage plants, industrial heat processes).

The project will revolve around the physics of supercritical fluids and how they can be applied to design novel zeolite-based nanoparticles and devices for energy storage purposes. For instance, new materials with thermo-mechanical energy storage capacity will be proposed. Here, the basic idea is to investigate and exploit the divergent heat capacity of a Super Critical water (sc H2O) by putting the scH2O in combination with an hydrophobic zeolite that acts as a pressure-volume buffer (molecular springs). In the case of electrochemical storage, the projects will continue our current research in "cheap batteries" by designing through scH2O technology specific zeolite based batteries with controlled nano-porosity.

Project S9. Next-generation single-chain nanoparticles (SCNPs) endowed with multiple functions

Contact person: José A. 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 next-generation SCNPs endowed with multiple functions such as catalytic properties, fluorescent activity and carrier capability. 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 S10. Non-equilibrium effects in superconducting hybrid structures with spin-orbit coupling

Contact person: Sebastián Bergeret (sebastian_bergeret@ehu.eus)

Hybrid structures containing superconductors and materials with strong spin-orbit coupling are the focus of several experimental and theoretical works, mainly due to the wide variety of

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applications that such systems may have in electronics, spintronics, and quantum computation. From a fundamental point of view, the interplay between superconductivity and spin-dependent fields leads to hitherto unknown effects that are being studying in different scenarios. However, most of the works in this research field focus on spectral and equilibrium properties of the systems. In the present project, we propose to theoretically study the non-equilibrium physics of superconducting hybrid structures with the main focus on materials with strong spin-orbit coupling and magnetic textures. The successful candidate will be trained in the quantum kinetic equations and Green's functions techniques, as well as on superconductivity and spin transport. From the candidate we expect basic knowledge in Condensed Matter Physics and mathematical methods in Physics.

Project S11. 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 S12. Surveying chemical reactions at surfaces and interfaces properties

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

The growing interest for organic-based materials derives from their potential in functional platforms for electrochemical energy conversion and storage system. This attractive potential emerges from the capability to form tunable, ordered and periodic structures with shape or chemical composition defined by the choice of molecular precursors. Yet, the material efficiency, its reactivity and charge transport are still challenging. Thus, reaching device applications requires a better understanding of the materials and interfaces at fundamental level. The present project addresses

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experimental questions at the joint frontier between surface physics and chemistry concerning the synthesis and characterization of organic interfaces. Here, we aim to clarify the fundamental aspects of metal-organic surface, such as the chemical reactions leading to molecular reactivity on surfaces, their electronic structure and stability towards charge storage/transfer and/or capability to promote catalysis. The characterization of these will be performed in ultra-high-vacuum using scanning probe techniques (STM, STS, AFM) at 1-Kelvin. These techniques will allow improving our knowledge on the synthesis of efficient organic layer for applications.

The candidate will acquire various 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 S13. Bringing functional molecular systems onto non-metallic surfaces

Contact person: Martina Corso (martina.corso@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 molecular carbon-based nanomaterials. In this challenging PhD project, several strategies will be explored to bring graphenic nanoscale materials onto non-metallic surfaces under ultra-high vacuum (UHV) conditions. The study of their structural and electronic properties will be done with surface sensitive characterization tools such as scanning tunneling microscopy/spectroscopy (STM/STS) and X-ray photoelectron spectroscopy (XPS). Specific graphenic nanoscale materials can be grown with atomic precision on metallic surfaces by means of on-surface synthesis. Nevertheless, the use of such materials as functional units in various technological applications as spintronics or optoelectroncis, requires non-metallic substrates as their support. In this PhD project both the direct synthesis on non-metallic substrates as well as transfer by atomic layer injection will be explored focusing on the study of the yet unexplored properties of nanographenes-transition metals dichalcogenides heterostrucutres and photopolymerisation on oxides. The successful candidate will be integrated in a multidisciplinary national collaborative project and in the international working environment of the NanoPhysics Laboratory.

Project S14. Novel Carbon-based Nanofluids for Energy Storage

Contact person: Félix Fernández (felix.fernandez@ehu.eus)

This project seeks to unravel the physico-chemical mechanisms underpinning the emergence of disordered and fluid phases in novel carbon-based materials, with a view to their use as a new

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platform for the storage of thermal energy. As such, it builds upon our recent work demonstrating the existence of genuine 'nanofluid' phases in fullerene derivatives, characterized by thermal-energy capacities comparable to top-performing (yet far-more complex) multicomponent materials. For the first time, this project will investigate unexplored strategies for the rational design of the thermophysical properties of these nanofluids, including the effects of curvature (and associated flexopolarity), flexibility of the chemical substituent, as well as the overall shape & symmetry of the molecular building blocks. The associated work plan will make extensive use of state-of-the-art neutron and X-ray instrumentation at leading international facilities, alongside computational materials modelling for a detailed interpretation of the experimental data at the molecular and supramolecular levels. We envisage that our results will pave the way for unprecedented insights into the untapped potential of this class of materials as novel media for the storage of thermal as well as chemical energy.

Project S15. Quantum effects in atomic-scale nanophotonics

Contact person: Javier Aizpurua (aizpurua@ehu.eus) and Rubén Esteban (ruben_esteban@ehu.eus)

This project aims at studying novel quantum phenomena in light-matter interaction, arising in systems that confine electromagnetic energy to nanometer and subnanometer regions. Localization of light well beyond the wavelength is usually not allowed in standard photonics due to the diffraction limit, but this limit can be overcome when collective electronic excitations, so-called plasmons, are effectively excited. Plasmons are usually studied within classical electromagnetic theory; however, nowadays it is possible to experimentally reach regimes of light-matter interaction where quantum effects become very relevant. The "Theory of Nanophotonics Group" at CFM, is pioneering a battery of theoretical methods to study quantum effects in nanophotonics. The person in charge of this project will develop, implement and apply many of these theoretical tools. Special attention will be devoted to the use of the cavity Quantum Electrodynamics (c-QED) formalism to describe the interaction between molecules and plasmonic structures, occurring at (sub)nanometer dimensions. The project aims at discovering and analyzing processes and phenomena only accessible thanks to state-of-the-art experiments in molecular spectroscopy and microscopy, including ultrafast spectroscopy, ultrahigh vacuum-low temperature tunneling microscopy, or photon emission correlation measurements. The candidate is expected to participate in ongoing collaborations of the group with other international groups.

Project S16. Machine Learning for Understanding Structure and Dynamics of Polymers and Biopolymers

Contact person: Gustavo Schwartz (gustavo.schwartz@csic.es) and Alejandro Miccio (luisalejandro_miccio@ehu.eus)

The objective of the work is to take a numerical route to determine the physical properties of polymers and biopolymers by using machine-learning techniques. This is currently a hot topic of scientific research and it is on line with the CSIC´s priority areas of research for the next decade. During the last years, considerable efforts have been spent in the development of Quantitative Structure Property Relationship (QSPR) models. Clearly, the possibility of predicting the behavior of novel materials (even before synthesizing them) and of understanding how structure and dynamics are related with the macroscopic physical properties is of utmost importance for materials scientists as well as for industrial applications. Among the many QSPR modelling methods, the use of artificial neural networks (ANN) has arisen as a very promising and suitable approach for establishing structure-properties relationships. Besides the ANN, we will also focus in this work on other numerical approaches (clustering, vectorization, PCA) in order to correlate the structure and physical properties of polymer-based materials as well as to shed some light into the understanding of the molecular mechanisms behind these behaviors. Only highly motivated candidates with very strong programming skills (preferably in Matlab) are encouraged to apply for this position. A basic background in polymer physics would be also desirable.

Project S17. Exploring Superconductor/Ferromagnetic Interfaces in quantum applications

Contact person: Celia Rogero (celia.rogero@csic.es)

We are looking for highly motivated PhD students with background in solid-state physics, superconductivity and magnetism to work in the framework of a multidisciplinary European Collaborative Project. Daily work will be conducted at NanoPhysics Laboratory, with frequent visits to synchrotron installations as well as to Nanogune.

We propose a challenging experimental PhD project, which endeavors to delve into the knowledge of certain quantum technological areas, in particular, those that arise from the coupling between a ferromagnetic insulator (FI) and a superconductor (S). The exchange field at the FI/S interface that leads to the splitting of the superconducting density of states can be exploited in applications such as thermoelectricity, superconducting spintronics, radiation sensors, quantum phase batteries, or non-volatile memory element. In this project, we will correlate the coexistence of this exchange splitting in S/FI structures with the layer-by-layer growth conditions, the interface quality and the use of conventional and novel materials. 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).

Project S18. Understanding catalytic reactions in-operando at the atomic scale: curved surfaces at ambient pressure

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

Catalysis is extremely important in industrial processes with notorious relation with energy and environmental problems. However, the most relevant catalytic reactions are still optimized following a trial-and-error philosophy. Further improvement requires a rational atomic-scale understanding through new sample designs and techniques that can bridge the gap with real catalyst materials. In a bid to model industrial nanoparticles in-operando, our Lab investigates curved metal surfaces exposed to millibar pressures of reactants, using novel atom-sensitive techniques that operate under such ambient-pressure conditions, such as X-ray photoemission.

The candidate will focus on the exploration of the structure and electronic properties of curved crystal surfaces, and their interaction with chemically active gases, such as CO, O2 and CO2, using Scanning Tunneling Microscopy and X-ray Photoemission in our laboratory. This work will be combined with Ambient Pressure X-ray photoemission experiments performed in Synchrotron Radiation facilities over the world to examine the interaction of millibar mixtures of reactants and products with such curved surfaces.

Project S19. Fundamental properties of magnetic topological insulators and their heterostructures

Contact person: Andrés Arnau (andres.arnau@ehu.eus) and Mikhail Otrokov (mikhail.otrokov@gmail.com)

Many applications, like sensing, data storage and quantum computation, are based on novel quantum phenomena that appear in two-dimensional magnetic materials. Its practical realization crucially depends on our ability to engineer and efficiently tune their electronic and magnetic structures. Among others, the atomic scale control of non-collinear spin textures in multilayer systems is expected to permit the development of race track memories and other devices based on the transfer of spin and orbital momentum when an electrical current flows across ferro- or antiferro-magnetic materials.

The aim of this project is to achieve a complete understanding of the electronic properties of several heterostructures made of two-dimensional magnetic materials, including topologically-

nontrivial two-dimensional systems. Special emphasis will be done on studying magnetic and relativistic phenomena, such as magnetic anisotropy, Dzyaloshinskii-Moriya interaction (in systems with broken inversion symmetry), and magnetic domain walls.

The candidate should preferentially have a Master in Physics, Quantum Chemistry, Materials Science or Nanoscience. Previous experience in one of the following areas will be highly valued: first-principles electronic structure calculations, computational materials science, tight-binding model Hamiltonians, Fortran and bash/tcsh programming. Good written and oral communication skills in English are required.

Project S20. In silico design of self-healing materials made of polymeric nanoparticles

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 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 simulations, the role of these factors on the formation and properties of reversible self-healing gels based on such objects. The simulations will be compared with experiments in systems available in the Polymers and Soft Matter Group of the CFM. 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. Quantum sensing based on levitated nanoparticles

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

The Quantum Nanophotonics Laboratory at Donostia, in the Material Physics Center (San Sebastian, Spain) is looking for highly motivated, talented researchers searching exciting opportunities to obtain a PhD in the area of Quantum Nanophotonics. The successful candidates will study both experimentally and theoretically the quantum dynamics of levitated particles. In particular, the successful candidate will investigate the use of these systems as magnetic and

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inertial sensors. Ideally, the candidate should already have a background in optical trapping or in quantum optics experiments. S/he will work in an optical set-up and integrate different experimental tools with Python or Labview.

The research environment consists on a strong team of researchers dedicated to control the properties of light at the nanoscale and the investigation of novel quantum effects in the interaction of light and particles. The Quantum Nanophotonics group at MPC is collaborating with renowned international research groups and companies to control the quantum properties of small material particles.