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, CFM is focused on the following research projects:

Project S1. *Nanostructured materials for artificial photosynthesis*

Project S2. *Hydrocolloids in foodstuffs – from mechanical to sensory properties*

Project S3. *Exploiting Atomistic Molecular Dynamics Simulations to Unravel Structural and Dynamic Properties in Different Aqueous Systems*

Project S4. *Dynamics of the CO-O recombination at metal surfaces studied from first-principles based on machine learning potentials*

Project S5. *Charge-Density-Wave Transitions in Topological Materials from First Principles*

Project S6. *Synthesis and electronic structure of one-atom-thick hexagonal boron nitride on curved crystals: toward boron nitride nanostripes*

Project S7. *Pressure induced topological transitions*

Project S8. *Generation of 1D/2D/3D optically active nano-microstructures by femtosecond-laser-induced processing of rare earth-doped glasses: spectroscopic characterization and performance*

Project S9. *Modeling of nano-composites based on two-dimensional materials like graphene*

Project S10. *Structure and dynamics of polymers: a multiscale approach*

Project S11. *Innovative Thermal Energy Storage (TES) solutions based on Near Supercritical Fluids (nSCF) with zeolite-based molecular springs*

Project S12. *Synthesis and characterization of new, well-defined single-chain nanoparticles (SCNPs) endowed with multiple functions*

Project S13. *Unconventional superconductivity in hybrid nanostructures*

Project S14. *Ultra-dense/low energy state glasses by aging nanostructured polymers*

Project S15. *Active control of plasmonic hybrid nanostructures*

Project S16. *Electron transport and chemical reactions on surfaces*

Project S17. *Dynamics of elementary reactive processes at two-dimensional materials*

Project S18. *Theoretical description of femtosecond laser-induced molecular desorption using abinitio molecular dynamics with electronic friction (AIMDEF)*

**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 http://cfm.ehu.es/activities-eventsworkshops/introduction/

7 PhD studentships available

Approximately 25 applicants will be shortlisted and invited for a 2-days visit to CFM in May 2019, with their travel and accommodation expenses fully covered. Personal interviews will be held and the candidates will have the opportunity to discuss the research projects with their supervisor.

From the interviews, 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. 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 2019 for the PhD contract to be continued. Therefore, **the candidates are required to hold a Master degree granted before the end of 2019**.

Application Process: The application process consists in filling an application in the following link http://cfm.ehu.es/cfm/index.php/phd-fair-2019

The following documentation is required for applying:

1. Fill in relevant data in the online 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 2nd April 2019, at 17:00 Central European Time (CET).

General complementary information: http://cfm.ehu.es/phd-recruitment-fair-2019/

Pre-Selection Process: The applications will be evaluated by an academic Evaluation Committee at CFM. It will be composed by Dr. Celia Rogero, Dr. Ivo Souza, Dr. Gabriel Molina-Terriza and Dr. Ángel Moreno, who will consider the CVs of the candidates, their background adequacy to the selected projects and the provided reference letters.

Only applications received before the deadline (2nd April 2019 at 17:00 CET) will be evaluated.

Final Selection Process: The list of pre-selected candidates will be published soon after at the CFM site (in the same announcement at http://cfm.ehu.es/about-cfm/job-offers), and they will be contacted personally for arranging their visit to CFM and agree a meeting for their personal interview. Soon after the visit, the academic committee will select the 7 awarded students and the final decision will be communicated to the applicants.

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

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LIST OF AVAILABLE PROJECTS

Project S1. Nanostructured materials for artificial photosynthesis

Contact person: Yury Rakovich (yury.rakovich@ehu.es) and Marek Grzelczak (marek.grzelczak@dipc.org)
Reference: PhD/2019/1

The control over the materials structure down to nanoscale as well as their electronic structure are the most important requisites to develop artificial photosynthetic systems that through photocatalytic conversion can efficiently store light energy in chemical bonds. Especially important is the nanomaterials composition that defines light harvesting capacity and drive catalytic reactions via electron transfer. The aim of this project is the rational design and development of a hybrid nanoparticle-based photocatalyst using variety of sub-units such as molecules, supra-molecular complexes, plasmonic nanoparticles and quantum dots to be later assessed on a single particle level with sub-particle resolution. 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 imaging as well as fluorescence correlation spectroscopy. The material development and advanced characterization techniques will serve to study the fundamentals of photocatalytic processes related to photosynthesis with special 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. Hydrocolloids in foodstuffs – from mechanical to sensory properties

Contact person: Silvina Cerveny (silvina.cerveny@ehu.eus) and Juan Carlos Arboleya (jcarboleya@bculinary.com)
Reference: PhD/2019/2

Oropharyngeal dysphagia is a condition involving perceived or real difficulty in moving food from the oral cavity to the esophagus. Although swallowing seems simple, it is actually a very complex activity, which involves motions of muscles, several nerves, esophagus, and brain activity. The prevalence of this disease increases with age and it is frequently observed in patients with dementia, including Alzheimer's disease and other neurodegenerative illness which affect over 7 million people in Europe, and it is expected to double every 20 years as the population ages. Texture modification of food is one of the most common ways of improving safe swallowing.
This thesis (included in the area of materials science) deals with the impact of solid and liquid consistency and food texture on swallowing. We will explore different types of hydrocolloids (pectin, starch among others) on foodstuffs and we will analyze their rheological properties using dynamic viscoelasticity measurements. Chemical and physical characterization of both

hydrocolloids and foodstuffs will be also done in order to correlate molecular parameters (glass transition, water activity, phase separation, crystallization, etc.) with the texture and viscosity of the food. In addition, in collaboration with the Bask Culinary Center, we will also correlate the rheological results with the perceived viscosity trough sensory evaluations.

Project S3. Exploiting Atomistic Molecular Dynamics Simulations to Unravel Structural and Dynamic Properties in Different Aqueous Systems

Contact person: Fernando Álvarez (fernando.alvarez@ehu.eus) and Juan Colmenero (juan.colmenero@ehu.eus)
Reference: PhD/2019/4

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 behaviour 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 S4. Dynamics of the CO-O recombination at metal surfaces studied from first-principles based on machine learning potentials

Contact person: Joseba Iñaki Juaristi (josebainaki.juaristi@ehu.eus)
Reference: PhD/2019/5

Recombination processes involving gas-phase and pre-adsorbed species on surfaces play a prominent role in a huge variety of natural and technological processes: in the production of chemical compounds, in the search for controlling the emission of noxious gases, and in the research on hydrogen storage, to just cite some relevant examples in which they are exploited from the catalysis perspective. In addition, these processes usually being highly exothermic, they are also known to be a major source of surface damage in general plasma-wall interactions, such as those occurring on the internal walls of fusion reactors or on aerospace vehicles during the atmospheric entry. In this project, we propose to investigate the recombination of O with preadsorbed CO. There are experiments showing that the efficiency of these process 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. The PhD candidate will acquire a strong background in theoretical chemical physics, including density functional theory, electronic structure calculations, molecular dynamics methods, scientific programming, and machine learning techniques.

Project S5. Charge-Density-Wave Transitions in Topological Materials from First Principles

Contact person: Ion Errea (ion.errea@ehu.eus) and Maia G. Vergniory (maia.garcia@ehu.eus)
Reference: PhD/2019/6

The goal of this project is to discover new topological materials, whose non-trivial topology can be controlled with temperature or strain. Such type of materials can provide a way of engineering devices where the robust properties of topological materials can be switched on/off.
We will make use of first-principles calculations to seek for materials with non-trivial topology that undergo a charge-density-wave (CDW) transition. A CDW is a structural phase transition that can modify the electronic properties. Since CDWs can be controlled with temperature and/or strain, materials undergoing CDW transitions are perfect candidates.
The phase diagram of candidate materials will be determined explicitly calculating the CDW transition temperature with the stochastic self-consistent harmonic approximation, which rigorously includes quantum and anharmonic effects, crucial in CDWs. We will also study the symmetry of the system and band topology of electronic states, as well as the gap functions when the CDW occurs.
The candidate will acquire a deep knowledge in advanced group theory, modern theory of topological materials, and phonon anharmonicity.

Project S6. 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) and Enrique Ortega (enrique.ortega@ehu.eus)
Reference: PhD/2019/7

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 S7. Pressure induced topological transitions

Contact person: Aitor Bergara (a.bergara@ehu.eus) and Aritz Leonardo (aritz.leonardo@ehu.eus)
Reference: PhD/2019/8

Pressure strongly modifies atomic structures of materials, resulting in highly complex physical behavior. For example, even though under normal conditions alkalies crystallize in simple compact structures, phase transitions to complex and low coordinated structures have been reported to emerge under pressure. Correlated to these transitions, a number of exotic phenomena arise under high pressure. For example, it has been shown that pressure enhances the superconducting transition temperature. Actually, last year two experimental groups observed that LaH10 superconducts at 260 K and 200 GPa, becoming the highest Tc ever measured.
On the other hand, topologically non-trivial materials (insulators, semimetals and metals) have become a hot topic in recent condensed matter physics research. Their electronic structures exhibit nontrivial band crossings near the Fermi energy. In this PhD project we propose to analyze possible pressure induced topological transitions even in simple systems, as a result of the already observed enhanced electronic complexity under pressure. Our group has spot more than 7000 topological materials, many of them present superconducting behavior under pressure. The study of the eventual connection between the topological transition and superconductivity will also be part of the research project.

Project S8. 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)
Reference: PhD/2019/3

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 S9. Modeling of nano-composites based on two-dimensional materials like graphene

Contact person: Andrés Ayuela (andres.ayuela@ehu.eus)
Reference: PhD/2019/09

Graphene oxide sheets are part of nanocomposite materials adding prospect functionalities based on the unusual properties of two dimensional materials such as mechanical stiffness and thermal conductivity for graphene. In this PhD thesis, we aim to study the structural, energetic and electronic properties of graphene oxide sheets taking part in new composites of inorganic materials interesting for today structures such as hydrated calcium silicates in cements or for biological purposes such as hydroxyapatite in bones. This PhD thesis would furthermore serve to bring into contact the two main topics in which are currently working with success in the group, namely two dimensional heterostructures and hydrated calcium silicates, which are at the core of cement research. This research would be interesting for the design of future energy storage applications in collaborations with other technological labs and international groups, which will be performing related experiments.
The tasks of the PhD students will be mainly to apply atomistic modeling to understand and predict the structural, energetic and electronic properties of graphene oxide sheets taking part in composites of inorganic materials using both first-principle and MD models. Experience with density functional theory (DFT) calculations as well as with the Fortran programming language will be highly valued.

Project S10. Structure and dynamics of polymers: a multiscale approach

Contact person: Ángel Alegría (angel.alegria@ehu.eus) and Daniel E. Martínez-Tong (danielenrique_martineztong001@ehu.eus)
Reference: PhD/2019/10

The development and future application of polymer-based technologies in key areas as environment, energy and healthcare, depends on our understanding of their basic physical properties. Specifically, a current challenge is centered around how the nanoscale structure and properties of polymers lead to the resulting bulk response. This problem relates to the spatial and temporal heterogeneities of these complex materials.
The aim of the PhD project is the study of the structure and dynamics of polymers, using a multiscale approach: from the macro- to the nanoscale. The student will carry out experiments using a wide variety of techniques available in our group. The research will be mostly focused on the study of molecular dynamics of polymers using Broadband Dielectric Spectroscopy (BDS), while the structural studies will be carried out via Atomic Force Microscopy (AFM) experiments. Moreover, taking advantage of the AFM lateral resolution, the student will engage into the

mapping of physical properties using this microscopy technique. This will allow the simultaneous characterization of topographical features and physical response of polymers at the nanoscale. Ultimately, we will aim towards providing unique means of linking structure to properties, study their relationship, and opening pathways for the development of more advanced materials.

Project S11. Innovative Thermal Energy Storage (TES) solutions based on Near Supercritical Fluids (nSCF) with zeolite-based molecular springs

Contact person: Jorge S. Dolado (jorge_dolado002@ehu.eus) and Elena Palomo (epalomo@cicenergigune.com)

Reference: PhD/2019/11

The proposed project aims at exploring a new idea with high theoretical and practical potential leading to a drastic change in the field of thermal energy storage (TES), providing an affordable-cost solution for ultra-compact storage achievement in a large spectrum of challenging applications (e.g. thermal power plants, concentrating solar power, compressed air energy storage plants, industrial heat processes). The basic idea is to investigate the possibility of exploiting the peculiar properties of a near Super Critical Fluid (nSCF) as a storage material, more particularly its divergent heat capacity. This property suggests that the energy storage capacity of the fluid becomes extremely large and increases while approaching the critical point, especially when isobaric transformations are used. However, under constant pressure working conditions significant volume changes are expected to occur in the nSFC during heating/cooling processes. This could be a limiting factor for fully exploiting the TES capacity of fluids near their critical point. To face this problem, the project will consider investigating the use of zeolite-based molecular springs, more specifically Porous Heterogeneous Lyophobic Systems (PHLS). It is well known that the infiltration/expulsion of a non-wetting liquid into/from a non-hysteretic condensed system of a nanoporous material is an isobaric process involving large volume changes. A conveniently designed PHLS, with infiltration/expulsion pressure close to the critical pressure of the nSCF and suitable porosity characteristics (size, amount, topology), should hence provide an easy solution for stabilizing the pressure and to manage the volume changes of the nSCF during the heating/cooling processes. As a result, the nSCF (as heat storage material) and the PHLS (as a pressure-volume buffer) could lead to a highly innovative TES technology providing unusually large storage capacity. The general objective of this PhD thesis is to provide the proof of the concept.

Project S12. Synthesis and characterization of new, well-defined single-chain nanoparticles (SCNPs) endowed with multiple functions

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

Reference: PhD/2019/12

The bioinspired folding/collapse of individual synthetic polymer chains to produce single-chain nanoparticles (SCNPs) is a field of intense activity. As a hot topic, we can mention the preparation of SCNPs mimicking either the function of intrinsically disordered proteins, e.g.

interaction with/transport of diverse substances, or the activity of enzymes, i.e. catalysis with high efficiency and selectivity. The present project aims to further advance the field of SCNPs by synthesizing new, well-defined SCNP systems endowed with multiple functions such as catalytic properties, fluorescent activity or carrier capability. An in-depth characterization of these new SCNPs 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 S13. Unconventional superconductivity in hybrid nanostructures

Contact person: Sebastián Bergeret (sebastian_bergeret@ehu.eus)
Reference: PhD/2019/16

Summary: The candidate will study spectral properties of superconductivity induced in different materials with arbitrary magnetic and electric properties. It is well know that a conventional superconductor when brought in electric contact to non-superconducting materials may generate in the latter superconducting correlations that might have a different symmetry from the conventional one. Such unconventional superconducting correlations may lead to interesting effects related to the transport of charge, spin and heat in nanostructures. This will be the focus of the candidate's status.
For that, the selected student will learn different analytic techniques used in theoretical condensed matter physics, which include Green's functions, Keldysh diagrammatic technique and scattering matrix approach.
We expect from the student a solid background in Solid State Physics and mathematical methods.

Project S14. Ultra-dense/low energy state glasses by aging nanostructured polymers

Contact person: Daniele Cangialosi (daniele.cangialosi@ehu.eus)
Reference: PhD/2019/13

This project takes inspiration from recent findings showing that glasses exhibiting large amount of free interface are able to access low energy states in remarkable short time scales. Hence, the thermodynamic state in these kinds of glasses – including polymer nanospheres, nanocomposites, thin films and foams – subjected to different thermal histories will be characterized. To do so, the PhD student will employ conventional and fast scanning calorimetry, that is, techniques providing access to the energy state of a given glass. Complementary techniques, such as broadband dielectric spectroscopy, will also be used. Exploring low energy states will allow producing ultra-dense glasses. This may result in a tremendous impact on the glass properties. Apart from this, the present project aims to clarify long-standing fascinating issues of glass science, such as the existence of the so-called "ideal" glass, that is, a disordered system with entropy equal to that of the corresponding ordered crystal.

We look for candidates with a background in experimental materials science. Candidates are expected to show a high degree of motivation and autonomy.

Project S15. Active control of plasmonic hybrid nanostructures

Contact person: Nerea Zabala (nerea.zabala@ehu.eus)
Reference: PhD/2019/14

Metallic nanostructures host electron collective oscillations (plasmons) when excited with light, allowing for confinement of optical energy to subwavelength volumes. Hybrid platforms combining metallic plasmonic nanoantennas and materials with special properties such as phase-changes, ferromagnetism, or spintronics, offer excellent technological opportunities for active plasmonics. The addition of ferromagnetic components strategically positioned into the noble metal structures allow for the fast and contactless actuation on the plasmon resonances using weak external magnetic fields, via the magneto-optical or magneto-refractive effects. The possibility of modulating the optical response using different plasmonic metasurfaces provides a very powerful route to new optical devices, as low-power and ultracompact optical modulators, switches or biosensors with increased performance and functionality.
The candidate will address theoretically the optical response of complex hybrid systems by using numerical simulation methods for solving Maxwell's equations. A background on electrodynamics, nanophotonics and computational methods will be highly valued.
This thesis project will be conducted within the Theory of Nanophotonics group and in collaboration with experimental groups at CFM, IMN-CNM in Madrid, Nanogune and University of Southampton.

Project S16. Electron transport and chemical reactions on surfaces

Contact person: Lucia Vitali (lucia_vitali@ehu.eus)
Reference: PhD/2019/15

The emission of carbon oxides generated by burning of fossil fuel for energy production is affecting global climate. In order to mitigate the negative effects of current energy sources both the reduction of carbon oxides in atmosphere and the development of alternative energy systems are pursued. Inverting the increasing trend with the capture and conversion of carbon oxides into hydrocarbons is a challenging option.
Despite the technical difficulties, natural photosynthesis performs daily these tasks starting from the absorption of sunlight. The transport of the photon-generated charges to the single-atom catalytic-sites is a necessary step to activate the redox reaction. Thus, the efficiency of an artificial system in capturing and promoting a redox reaction relies on both the energy input and the catalytic site.
In this project, scanning probe techniques will be used to address the adsorption and reaction of gas molecules on (metal)-organic network. These techniques have demonstrated to be essential in the characterization of both the electron-transport and reaction mechanism in surface-supported heterogeneous-catalysis. The main question to be addressed concerns the

reactivity of the organic network, which will be surveyed according to the functional groups/atoms, their chemical environment and electronic properties of the surface supported structure.

Project S17. Dynamics of elementary reactive processes at two-dimensional materials

Contact person: Ricardo Díez Muiño (rdm@ehu.eus)
Reference: PhD/2019/17

Advances in the description of elementary reactive processes at surfaces are largely triggered by the quest for systems and conditions under which reactivity can be controlled, enhanced or inhibited. From this point of view, two-dimensional (2D) layered systems, such as transition metal dichalcogenides or transition metal carbides/nitrides, are receiving increasing attention due to their high activity as catalytic agents. The catalycity of these systems can be also very dependent on the presence of defects as well as on the nanostructural properties when the system is finite (nanoribbons, nanosheets, etc.). The goal of this project is to advance in the theoretical description of physico-chemical processes that involve the interaction between small molecules (H2, N2, CO, NO, O2…) and 2D materials. Ab-initio molecular dynamics (AIMD) based on density functional theory (DFT) and dynamics based on machine-learning potentials will be used to describe the dynamics of adsorption and dissociation processes. The PhD candidate will acquire a strong background in theoretical chemical physics, including density functional theory, electronic structure calculations, molecular dynamics methods, scientific programming, and machine learning techniques.

Project S18. Theoretical description of femtosecond laser-induced molecular desorption using abinitio molecular dynamics with electronic friction (AIMDEF)

Contact person: Maite Alducín (maite.alducin@ehu.eus)
Reference: PhD/2019/18

Femtosecond laser induced desorption has been experimentally demonstrated to be a promising technique to trigger and control the recombination and reaction of adsorbates on surfaces. However, the complexity and variety of the physical processes involved (electron excitations, surface phonons, adsorbate's excited states) and the strong dynamical nature of all of them have limited our understanding of the variables determining the efficiency and applicability of this technique. The new AIMDEF methodology that accurately accounts for the electronic and phononic excitations, which is also computationally efficient, is perfectly fitted to investigate existing unsolved issues. The objective of the project will be to investigate, using this methodology, different laser induced adsorbates reactions of practical interest (e.g., recombinative desorption of H_2, CO_2, NO_2, desorption of CO, NO, diffusion, etc.) and disentangle the role and efficiency of the laser-excited electrons and the concomitant electron-excited phonons in the whole process. The PhD candidate will acquire a strong background in theoretical chemical physics, including density functional theory, electronic structure calculations, molecular dynamics methods, scientific programming, and machine learning techniques.