Donostia International Physics Center

DIPC PhD STUDENT GRANTS

The Donostia International Physics Center DIPC is currently accepting applications for PhD students. This is a unique opportunity for highly motivated students, recently graduated from the University in physics or related fields, to develop a research career joining some of the DIPC high-profile research teams.

DIPC PhD grants last for just 12 months. An extension of the grant may be accepted just in some exceptional cases. DIPC PhD grants are intended to support the student during the first steps of his/her research career. Further financial aid to continue the PhD research project after this period should be obtained from other institutions.

Interested candidates please send an updated CV including an academic transcript with the obtained marks, a brief statement of interest, and contact information to phd@dipc.org. Reference letters are welcome but not indispensable. The particular PhD position(s) to which the candidate is applying should be stated as well.

Applicants are advised to hold, or be in the final year of a master's degree in physics, chemistry or material science.

Next review of applications is scheduled for July 20th 2018. Applications will be evaluated by a Committee designed by the DIPC board on the basis of the following criteria (with point weights indicated in parentheses):

- CV of the candidate (60%)
- Adequacy of the candidate's scientific background to the project (20%)
- Statement of interest and reference letters (10%)
- Others: Diversity in gender, race, nationality, etc. (10%)

Evaluation results will be communicated to the candidates soon after. Positions will only be filled if qualified candidates are found.

The DIPC could revoke its decision in case the candidate breaches the condition of joining before the deadline indicated in this call, proceeding in that case to grant the position to the next candidate based on the classification order, and provided that he has obtained a score higher than 50 (out of 100) in the evaluation of his candidature.

However, the selected candidate may keep the position if, in the opinion of the Evaluation Committee, he duly justifies the reasons why he can't join before the specified deadline, and as long as the project allows it.

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PhD OPENINGS

- Intrinsically disordered drug discovery

Contact person: David de Sancho (david.desancho@ehu.eus). Reference: 2018/15.

In the last decade, intrinsically disordered proteins (IDPs) have received widespread attention due to their abundance and their prevalence in cellular signalling networks. Lacking a well defined three-dimensional structure, IDPs are able to sample broad ensembles of conformations that have been characterised using structural biology techniques but also modelling and simulation. IDPs are also very important in disease. Here we will focus on a particularly important system, the hypoxia inducible factor HIF-1α and its homolog CITED2, both of which are IDPs. They regulate the cellular response to hypoxia, a common condition in many cancers due to the difficulty of oxygen diffusion in primary tumours and their metastases. We propose exploiting the conformational dynamics of HIF-1 to inhibit the binding to its cellular target, the CREB binding protein (CBP), as a new avenue for drug discovery. We will use molecular modelling and simulation technique to shed light on the mechanism of the binding of HIF-1α and its displacement by CITED2. Once we characterize the binding properties in the ternary complex we will develop small peptide analogues of CITED2 in order to develop therapeutic applications. The outcome of this project will provide proof of principle for a radically new drug discovery strategy that exploits the competitive advantages in the binding of disordered proteins.

- *Molecular Dynamics Simulations of femtosecond laser induced desorption of adsorbates from metal surfaces*

Contact person: Iñaki Juaristi (josebainaki.juaristi@ehu.eus) and Maite Alducín (maite.alducin@ehu.eus). Reference: 2018/16.

Femtosecond laser pulses in the ultraviolet and visible wavelength range constitute an efficient tool to promote reactions, diffusion and desorption of adsorbates at surfaces. In the case of metallic surfaces, the excitation of the adsorbates is indirect. The process is initiated by the excitation of the electronic system that is driven out of equilibrium. Subsequently, the electronic system can transfer energy directly to the adsorbate or to the phonon system by electronphonon coupling. As a consequence, the energy transfer between the metal and the adsorbate that promotes the reactions can be electron and/or phonon mediated.

The aim of this PhD project is to perform molecular dynamics simulations that can allow to reproduce and comprehend experimental results for several adsorbate/target combinations. The evaluation of relative role played by the electronic and phononic excitations, the quantitative description of interadsorbate energy exchange and the investigation of coverage dependent effects are among the objectives of the project.

The methodology to be used involves electronic structure calculations based on density functional theory, abinitio molecular dynamics, generation of potential energy surfaces with machine learning techniques and time dependent density functional perturbation theory among others.

- Exotic magnetism and electron-correlation phenomena at the interface of rare-earth based materials and molecular overlayers

Contact person: Frederik Schiller (frederikmichael.schiller@ehu.eus).
Reference: 2018/22.

The project addresses magnetic properties as well as electron-correlation phenomena at the interface of rare-earth (RE)-metal compounds and molecular overlayers. RE-metal compounds are generally known to exhibit a wide variety of unusual properties, caused by the delicate interplay of electronic and magnetic degrees of freedom, such as magnetic order via superconductivity, or Kondo and heavy-fermion behavior. Such phenomena are traditionally discussed for the bulk of the systems, but may become radically different at the surface, where also novel properties arise. In reality, all the aforementioned properties of RE-metal compounds arise from the delicate interaction of the localized 4f electrons with the extended Bloch-states of the valence band, which depends on symmetry properties and energy positions of valence band states, and hence on the composition and structural properties of the compounds. Valence states can be readily varied at the surface, for example, by alloying or deposition of adlayers, and be straightforwardly probed by means of surface sensitive techniques. Within this work ordered molecular overlayers will be investigated for this purpose.

The candidate will focus on RE-based compounds (RE = Sm, Eu, Gd, Ho and Yb) within RE-noble metal single-layer alloys RE-NM2 (NM = Au, Ag), where the rare-earth material can be encountered completely at the topmost atomic layer, and the materials are synthesized by in-situ deposition. Furthermore metal-centered semiconducting molecules will be deposited on top of these surface compounds with the aim to modify the elelctronic and magnetic properties. The work comprises (i) the synthesis of these materials and the characterization of their structural properties. Further characterization is carried out spectroscopically, by (ii) angle-resolved photoelectron spectroscopy (ARPES) in the UV and soft X-ray range, as well as magnetically (iii) by Magneto-Optic Kerr Effect and X-ray Magnetic Circular Dichroism, and theoretically, through (iv) band structure calculations in collaboration with theory groups of DIPC.

- Protonic conductivity mechanism in new electrolytes based on strong acid hydrate.

Contact person: Daniel Sanchez Portal (daniel.sanchez@ehu.eus) and Arnaud Desmedt (arnaud.desmedt@u-bordeaux.fr)
Reference: 2018/23.

Designing new devices dedicated to energy storage and production is at the center of nowadays concerns. Fuel cells constitute one attractive alternative and the nature of the electrolyte composing their proton exchange membrane is a central issue. It has been recently shown that new opportunities are offered by solid electrolyte composed of Strong Acid Clathrate Hydrates – nanoporous ice-like materials in which anionic guest molecules are included into a cationic host water cage structure. This confinement leads to generate proton excess delocalized along water molecules of the cage network, at the origin of their super-protonic conductivity overlapping those of utilized polymeric membrane (e.g. Nafion). The hydration number (i.e., the molar ratio of water to strong acid) plays a key role onto the protonic conductivity, the thermodynamic stability and the microstructuration of this new solid electrolyte. The driving factors at the origin of these properties are lying at a molecular and ionic level (e.g., adsorption sites of the guest molecule, Brownian dynamics of the various chemical species), for which a fundamental understanding is required. The present PhD project aims at understanding the elementary mechanism at the origin of this super-protonic conductivity and its hydration number dependence by combining experimental and theoretical strategies. The candidate will focus on strong acid hydrates (e.g., perchloric acid, hexaflurophosphoric acid, etc.) known to have the best protonic conductivity and thermodynamic stability. The work comprises (i) the synthesis of these materials for various hydration numbers with a recently established protocol. Experimentally, the formed hydrates will be investigated by (ii) synchrotron X-ray diffraction and Raman imaging for revealing their structural properties at atomic scale and their microstructuration, and (iii) by quasielastic neutron scatteing for unraveling their proton dynamics. The theoretical approach comprises (iv) the modeling of the strong acids adsorption site in the water cage (binding energies, crystallographic positions, etc.) by means of DFT calculations, followed with (v) “on the fly” Molecular Dynamics (MD-DFT) for unraveling the protonic transport mechanism. This project will be development within the framework of the Transborder Lab “Quantum Chem Phys” initiative and, thus, it will offer the opportunity for the student to spend 1.5 year at DIPC-San Sebastián for the theoretical part and 1.5 year at ISM, Univ. Bordeaux for the experimental part.

- Axionic Wave Dark Matter Project

Contact person: Tom Broadhurst (tom.j.broadhurst@gmail.com). Reference: 2018/29.

The student will investigate predictions of the light axion model of dark matter, via new simulations and with new observations. This is a joint theory and experimental project aimed at distinguishing between standard heavy particle dark matter (WIMPs) and wave-like axionic dark matter motivated by String Theory. The student must be prepared to reduce data imaging data from the Hubble Space Telescope and spectroscopy from the GTC telescope on La Palma. Travel to Taipei (NTU) and Hong Kong (HKU and HKUST) will be required to further the simulation work (in collaboration with Smoot, Tye, Chiueh and Schive), with coding required in CUDA on GPU clusters and continuation of theoretical work is needed with our current collaborators in Harvard (in collaboration with Emami).

- Optical phenomena in novel Van der Waals materials

Contact person: Alexey Nikitin (alexey@dipc.org). Reference: 2018/30.

Over the past decade, there is a growing research activity on light-matter interactions in atomically thin materials, such as graphene, topological insulators, thin polar and semiconducting layers and other Van der Waals materials, including their heterostructures. However, light-matter interaction in low dimensions is still a rather unexplored field, with an ample room for studying both basic fundamental concepts and potential relevant applications. The offered PhD project aims at the exploration of the optical phenomena in newly emerging Van der Waals materials by combining both experimental (far-filed spectroscopy and near-field optical microscopy) and theoretical (numeric simulations and analytical modelling) approaches. The project will study the fundaments of the propagation and excitation of light in atomically-thick Van der Waals materials (particularly in graphene, polar dielectrics and their heterostructures) and develop the concepts for using these materials in opto-electronic and photonic applications, such as e.g. extremely thin photodetectors, sensors, polarizers and absorbers. The experimental part of the project will be realized in a close collaboration with Nanogune research center. A close daily contact with experiments performed with the help of a state-of-the-art equipment will allow the PhD student to work on the very frontiers of science.