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 January 26th 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 does not join his/her duties within 6 months after the publication of the list of selected candidates.

Donostia International Physics Center

PhD OPENINGS

- Computational condensed matter physics: Electronic excitations in organo-metallic compounds

Contact person: Peter Koval (peter_koval@ehu.eus). Reference: 2018/1.

There is one PhD position in the Simulation and Modelization group at Centro de Fisica de Materiales and Donostia Int. Phys. Center. The successful candidate will work on the development of an efficient methodology to predict/simulate the excitation spectra of complex systems where spin degrees of freedom become important, like large organo-metallic complexes relevant in photovoltaics and nanoelectronics or new 2D materials like dichalcogenides. We are employing Hedin's GW approximation (GWA) followed by a solution of Bethe-Salpeter Equation (BSE). The GWA/BSE methodology goes beyond standard approaches of density-functional theory (DFT) and time-dependent DFT (TDDFT) and provides a description of the electron excited states comparable to wave-function-based methods such as "golden standard of quantum chemistry" --- coupled-cluster approximation.

The work will be performed under the supervision of Dr Daniel Sanchez-Portal and Dr Peter Koval, in a collaboration with Prof. Andres Arnau (UPV/EHU, San Sebastian, Spain) and Prof. Roland Hayn (IM2NP, Marseille, France). The student will apply and develop ab-initio methods to simulate the electronic structure and excited states properties of finite and extended systems within the framework of numerical atomic orbitals (NAO). NAOs are widely used in quantum mechanics/molecular mechanics (QM/MM) simulations because they make possible a parsimonious description of the electronic degrees of freedom allowing for a fast solution of the constituents described with QM.

We are looking for a motivated candidate with a background in condensed matter physics, interest in materials theory, good command of written and spoken English. A knowledge of electronic structure methods (DFT/Hartree-Fock) is essential. A familiarity with modern programming languages such as Python, Fortran, C/C++ is desirable.

- QM and QM/MM simulations of phosphate hydrolysis reactions catalized in various environments.

Contact person: Xabier López (xabier.lopez@ehu.es). Reference: 2018/2.

Phosphate hydrolysis reactions are ubiquitous in biology, and they are at the center of various key biochemical reactions in the cell. The role of the metals in the catalysis of these reactions have received considerable attention in the literature, but it is still not fully understood. Computational methods help in predicting the role played by metals and metal oxides in the activation of these important reactions. The goal of this project is to use QM and QM/MM methods to determine the reaction mechanism of phosphate hydrolysis in the presence of various metal and metal oxides. The theoretical predictions will be compared with available experimental data, and they will allow to put in a firm theoretical bases the catalytic ability of metals for this important set of biological reactions.

- Electronic and thermal transport through strongly correlated systems as described by density functional theory

Contact persons: Stefan Kurth (stefan.kurth@ehu.es), Roberto D'Agosta (roberto.dagosta@ehu.es). Reference: 2018/6.

We are currently looking for a motivated PhD student to work on the theoretical development and implementation of a Density Functional Theory for the description of electronic and thermal transport through strongly correlated systems. The aim of the project is to study how strong electronic correlations, e.g., in the Coulomb blockade regime of molecular electronics, affect the transport coefficients. Previous results show that this effect can be significant and can potentially open the way to novel materials for thermoelectric applications. The project also aims at implementing this novel theory into some widely distributed numerical code for electronic transport calculations.

The candidate should hold a Master Degree in Physics and ideally have some basic knowledge of density functional theory and other electronic structure methods.

- Dynamic self-assembly of plasmonic nanoparticles in flow

Contact person: Marek Grzelczak (marek.grzelczak@dipc.org).
Reference: 2018/7.

Liquid-phase self-assembly of plasmonic nanoparticles is a tool for the fabrication of novel stimuli-responsive materials with enhanced light harvesting capacity, a feature relevant for photocatalysis or biosensing. Experimental task of obtaining proper spatial distribution of nanoparticles is by now very challenging due to a number of principal physico-chemical limitations of the self-assembly process. One of emerging, yet highly unexplored approach to this challenge is an adaption of self-assembly from batch to flow conditions using, for example, microfluidic technology. Flow conditions enable the implementation of real-time analytics that improves experimental control, thereby enhancing the homogeneity of the new materials and resulting optical response.

The aim of this PhD program is the development of microfluidic system equipped with real-time spectroscopy for the self-assembly of the plasmonic nanoparticle using biomolecules (DNA, proteins) as stimuli and elaboration of corresponding synthetic protocols. The research program will involve collaboration with Electron-Microscopy Lab at CIC nanoGUNE in a part of real time in-situ monitoring of self-assembly.

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, self-assembly, plasmonics, surface chemistry, Microfluidics, biochemistry. Programming skills in Python would be an advantage.