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 May 19th 2017. 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.

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PhD OPENINGS

- Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics

Contact person: J. Aizpurua and R. Esteban (aizpurua@ehu.eus, ruben_esteban@ehu.eus). Reference: 2017/4.

Metallic nanoparticles support strong resonances at optical frequencies called plasmons, which can confine light to extremely small volumes and thus present very efficient coupling with nearby molecules. The properties of these plasmonic nanocavities have been studied using mostly a classical framework based on Maxwell's equations. There is, however, a growing interest on understanding how quantum effects such as electron transfer processes, the atomistic configuration of the system or the quantized nature of plasmons and molecular transitions influence the plasmon-molecule interaction.

The student will work in the Theory of Nanophotonics group (http://cfm.ehu.es/nanophotonics) to develop and apply quantum methodologies to better understand the physics behind the plasmon-molecule interaction, and how controlling this interaction may impact applications in fields such as spectroscopy, optoelectronics or quantum information. The methodologies to be considered can be based on Quantum Electrodynamics (QED), Time-Dependent Density Functional Theory (TDDFT) and other approaches. This work can be complemented with an analysis based on classical or semi-classical theories. Of particular interest could be the study of the behavior of molecules situated at very narrow gaps between metallic particles, as this situation combines effects linked to very large coupling strengths, strong field inhomogeneities, electron-transfer and chemical interactions.

The work will be theoretical, but the group works with many experimental groups and the student is expected to contribute to such collaborations whenever possible. The student is also expected to work closely with other theoreticians experts on topics closely related to the present work, as for example quantum modeling of materials, quantum information or quantum chemistry. The candidate should be willing to perform stays of up to several months with our collaborators worldwide. A strong background on nanophotonics, quantum optics, ab-initio modeling of materials and/or QED will be particularly valuable.

Depending on funding, one or two candidates will be selected.

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- Lifetimes of HOMO and LUMO states of organic molecules relevant for organic photovoltaics on different substrates

Contact person: D. Sanchez-Portal (daniel.sanchez@ehu.es). Reference: 2017/5.

The overall goal of this PhD project is to theoretically investigate the electronic structure of organic molecules attached to different relevant substrates using a combination of density functional theory (DFT) and/or many-body perturbation theory (GW-BSE) techniques. The focus will be in the calculation of both elastic and inelastic lifetimes of the frontier orbitals of such adsorbed molecules. In this project, code/method development and part of the applications will be performed at CFM-CSIC in San Sebastián, Spain, while some specific applications of the method will be performed at the University of Milano-Bicocca, Italy.

Candidates who have a previous Master's degree in a field relevant to the mentioned PhD-project may seek the fellowship (physics or theoretical chemistry). Candidates should have an excellent background in solid-state physics, density functional theory and basics of many-body perturbation theory.

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- Development of Density Functionals

Contact person: E. Matito (ematito@gmail.com). Reference: 2017/6.

Density Functional Theory (DFT) has found applications on a wide variety of scientific areas due to its remarkable combination of efficiency and accuracy. It is being applied with success to the fields of bioinorganic chemistry, material science, drug design, biochemistry and nano-technology, among many others. The exact density functional expressions of many energy components have not been found, and as a result, the construction of new functionals in DFT has become a complicated task, often untangled by the recourse of fitting parameters with the aid of experimental results. In this regard, the errors in DFT calculations are hardly predictable and for each new scientific challenge functionals must be calibrated against the expensive standard ab initio methods to assess their performance. DFT has reached a state of saturation, and the design of new strategies for constructing DFT functionals is now of utmost importance.

In this work, the goal of PhD student will consist in the design density functionals for the calculation of nonlinear optical properties (NLOP), which will lead ultimately to an all- urpose functional yielding reasonably accurate results in many applications. To this aim, several tools developed in the group will be used in order to identify the prime ingredients of DFT functionals. The theoretical work will be carried in the DIPC in close collaboration with the group of Dr. Josep M. Luis at the Univ. of Girona. Expertise in programming (Fortran preferred), solid background in DFT and knowledge of Mathematica software will be highly valued.