Donostia International Physics Center

DIPC - PhD GRANTS

The Donostia International Physics Center (DIPC) is currently accepting applications for PhD students. This is a unique opportunity for highly motivated students 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.

More information on these positions can be obtained by contacting: phd@dipc.org.

Deadline for applications is scheduled for April 3rd.

The available PhD research projects are described below.

Donostia International Physics Center

PhD OPENINGS

- ***Electron transport in nanostructures***

Contact person: Dr. Aran Garcia-Lekue (wmbgalea@lg.ehu.es)
Reference: 2013/2

In the last years, quantum electron transport through nanostructures has attracted great interest as nanoscale junctions or molecular devices may create a molecular electronics technology in the future. The current flowing through a nanostructure can be measured using scanning tunneling microscopy (STM) and breakjunction techniques.

The objective of this project is to simulate electron transport in nanostructures, from single molecules to self-assembled monolayers, sandwiched between metallic electrodes. Such calculations are aimed aimed at the prediction and/or understanding ofexperimental observations.

We will consider elastic transport, as well as inelastic transport due to the excitation of vibrational modes of the molecule. We will start by looking at the geometry and structure of different nanostructures on metallic surfaces, then continue studying fine spectroscopic details. First principles methods based on density functional theory (DFT) will be employed for the structural optimization, electronic structure characterization and calculation of vibrational modes. For the electron transport simulation, either non-equilibrium Green's function formalism or scattering-states method will be used.

- ***Non-adiabatic effects in the interaction of metal surfaces with atoms and small molecules***

Contact person: Dr. Maria Blanco Rey (maria_blancorey@ehu.es)
Reference: 2013/3

Heterogeneous catalysis is a recurrent motivation in surface science. Many molecules that are highly stable in their gas phase, e.g. N_2 or O_2, show a reduced binding energy upon interaction with a metal surface, specially when colliding at hyperthermal velocities. The case of atomic species is equally interesting, because the inverse process, i.e. selective molecule formation, can take place. Such a synthesis process may release a large amount of energy onto the surface, and therefore it is considered to be a major source of damage in aerospace vehicle coating materials, which perform in environments where ions and single atoms are present.

We propose to study the dynamics of such interactions. First principles calculations based in the Density Functional Theory (DFT) are a useful tool in this field, since they provide with accurate quantitative information in problems of high sensitivity towards multidimensionality, as it is the case of molecule/atom-surface interactions. Nevertheless, usual DFT calculations do not feature built-in non-adiabatic effects, but they are usually introduced “a posteriori” in the dynamical analysis using a number of parametrizations. Non-adiabatic effects account for the vibrational (phonons) or electronic (electron hole pairs) excitations on the surface brought by the aformentioned energy exchange. In the proposed project, we will explore several implementations of these energy loss channels, as well as their application to relevant case studies.

- ***Low-energy collective electronic and spin excitations in quasi-2D metallic systems***

  Contact person: Dr. V.M. Silkin (vyacheslav.silkin@ehu.es)
  Reference: 2013/5

  The aim is to carry out first-principles calculations of the dielectric response properties in a variety of quasi-2D materials like graphite intercalated compounds and topological insulators in the framework of the Time-Dependent Density-Functional Theory. The goal of this project is to determinate the role of the energy bands in the vicinity of the Fermi level in the formation of the low-energy electronic and spin collective excitations in these systems. Experience with first-principles density-functional methods is desired.