Donostia International Physics Center

# DIPC VISITING SENIOR RESEARCHER

The Donostia International Physics Center DIPC is currently accepting applications for one full-time visiting senior researcher appointment.

Interested candidates please send an updated CV, a brief statement of interest, and contact information to senior@dipc.org. The particular position(s) to which the candidate is applying should be stated as well. Please be aware that the application will be evaluated only if it is submitted directly to the email address mentioned above (senior@dipc.org).

Next review of applications is scheduled for April 10th 2015. Applications must be received before this date and 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 (45%)
- Adequacy of the candidate's scientific background to the project (45%)
- 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 duration of the appointment will be 10 months.

The salary will be determined in accordance with the DIPC salary plan and the applicants' education and research experience.

Donostia International Physics Center

# JOB OPENINGS

- ***Charge and spin transfer at nano-interfaces. Reformulation of Marcus theory using the molecular polarizability as fundamental variable.***

  *Contact person: J. Ugalde (jesus.ugalde@ehu.eus). Reference: 2015/2.*

  Work will focus on two topics that complement each other, namely, the theory of charge and spin transfer in nano-interfaces and a reformulation of electron transfer theory using the molecular polarizability as the fundamental variable.

  (A). Transient dynamics of interfacial charge and spin transfer

  Here the idea is to work out a theoretical model for the description of the transient dynamics of charge and spin transfer in nano-interfaces consisting of a nanoparticle and an adsorbed chiral molecule. The objective of this analysis is to unveil the physics of the formation of magnetic dipoles due to a transient solenoid effect where spin and linear momentum are coupled due to the transport process in the chiral structure. This investigation could have an important impact in the area of nano-magnetism and also in allowing us to gain a deeper understanding about the recently discovered Chirality Induced Spin Selectivity (CISS) effect and the role of spin in biological electron transfer.

  A description of this type of electron dynamics requires the use of a correlated quantum theory as time-dependent DFT to include the local field effects that does not currently exists.

  (B). Reformulation of Electron Transfer Theory in terms of dielectric response and molecular polarizability

  Electron transfer is one of the most important processes in chemistry and biology. Most of the earlier formulations in the literature are based on Marcus theory which is formulated in the energy representation domain, where the coupling between the electronic states involved in the transfer is a key ingredient. Unfortunately, the calculation of this electronic coupling requires of a number of arbitrary assumptions about the initial and final molecular orbitals involved in the transfer that makes the theory less robust than desirable. One alternative can be using the molecular polarizability and time-dependent fluctuations of the dielectric response as a way to reformulate the theory in terms of a time-dependent electronic density subject to fluctuations induced by changes in the nuclear polarization of the solvent.