

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 October 31st 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.

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.

PhD OPENINGS

- Relaxation of electronic states of magnetic add-atoms at surfaces considering Numerical Renormalization Group (NRG).

Contact person: Asier Eiguren (asier.eiguren@ehu.eus), I. G. de Gurtubay (idoia.gurtubay@ehu.eus). Reference: 2017/14.

We are currently looking for a PhD student in the field of Condensed Matter Physics and first principles calculations to carry research on the dynamical processes of charge and spin states on add-atoms including correlation effects beyond perturbative methods.

The candidate should have a Master in Condensed Matter Physics. Experience in the use of ab-initio electronic structure calculations and basic knowledge of Green's functions is highly desirable.

- Looking for new fermions in conventional crystals

Contact person: Aitor Bergara (a.bergara@ehu.eus) and Maia Garcia Vergniory (maia.garcia@ehu.eus). Reference: 2017/15.

Very recently Bradlyn et al. (Bradlyn et al. Science 353, 6299 (2016)) suggested that non symmorphic crystals could show a new family of topologically protected fermionic quasiparticles. We are currently looking for a PhD in the field of theoretical and computational physics to apply the chemical/physical topology described in the article above to find ideal materials with such interesting properties. Once we have found them, we will also characterize the modification on their physical properties when a symmetry breaking external deformation is applied.

Candidates should be motivated students with a strong background in condensed matter physics. Previous knowledge on topological physics is also preferred.

- Study of Intracule Functions

Contact person: *Eduard Matito* (ematito@gmail.com), *Xabier Lopez* (xabier.lopez@ehu.eus). 2017/16.

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 study of intracule functions of the pair density and find appropriate expressions to develop new DFT functionals. These functionals will be also tested for the performance of time-depedent DFT calculations of charge-transfer complexes. 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. Expertise in programming (Fortran o python), solid background in DFT and knowledge of Mathematica software (Mathematica, Matlab, Maple, etc.) will be highly valued.

- TDDFT approach for the direct calculation of exciton binding energies

Contact person: Aritz Leonardo (aritz.leonardo@ehu.eus). 2017/21.

The precise and efficient calculation of excitonic properties is an important task of computational materials science. The design of novel photovoltaic materials for instance, rely on this type of calculations to enhance the power conversion efficiency.

We are currently looking for a PhD in the field of condensed matter physics and first principles calculations to carry research on the calculation of exciton binding energies of extended systems within the linear response TDDFT formalism. A strong background on theoretical condensed matter physics, as well as, experience in the use of ab-initio electronic structure calculations will be highly valued. Fortran programming skills are not required but desirable.