

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 5th 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 breaches the condition of joining before the deadline indicated in this call, proceeding in that case to grant the position to the next candidate based on the classification order, and provided that he has obtained a score higher than 50 (out of 100) in the evaluation of his candidature.

However, the selected candidate may keep the position if, in the opinion of the Evaluation Committee, he duly justifies the reasons why he can't join before the specified deadline, and as long as the project allows it.

PhD OPENINGS

- PhD in Quantum Nanophotonics

Contact person: Gabriel Molina (gabriel.molina.terriza@gmail.com).

Reference: 2018/31.

The successful candidates will study both experimentally and theoretically the interaction of quantum states of light with subwavelength structures, such as plasmonic nanoantennae, quantum dots and nanodiamonds. The Quantum Nanophotonics group at MPC is collaborating with renowned international research groups to control the quantum properties of small material particles. We are also collaborating with industrial partners to make them suitable to become the next generation of biosensors or to perform very precise measurements of electric and magnetic fields.

In this project, the PhD candidate will operate a closed-loop cryostat in order to measure how the transfer of quantum correlations from light to small particles can be controlled. The candidate will also work on the generation of quantum states of light and the classical characterization of the scattering from nanostructures.

- Triplet states in PDI and related organic molecules

Contact person: David Casanova (david.casanova@ehu.eus), Jon M. Matxain (jonmattin.matxain@ehu.eus).

Reference: 2018/34.

Perylene-3,4:9,10-bis(dicarboximide) (PDI) and its derivatives are well known visible organic chromophores with excellent optoelectronic properties for energy and charge transport [1]. Moreover, their molecular rigidity results in robust thermal and photochemical stabilities and strong absorption capabilities of visible and near-infrared (NIR) light. Photophysical properties of PDI aggregates are of special interest as light-harvesting materials in organic photovoltaics [2].

While low-lying singlet excitations of PDI have been largely investigated, much less is known about the triplet state. Despite that the triplet manifold is not initially accessible through photoexcitation, recent studies have identified spin triplets as the final photoproduct states upon exciton decay processes in PDI dimers [3] and in the crystal [4].

We are looking for a PhD student in the field of theoretical and computational chemistry in order to unravel the properties of the lowest triplet state (T_1) in molecular and crystal PDI, and related species. She/he will describe in great detail the electronic structure of T_1 and rationalize the particularities of the triplet manifold in the crystal structure by means of computed vertical energy gaps, exciton delocalization, interchromophoric interactions and charge transfer contributions. To that end, she/he will make use of a variety quantum chemistry methods and computational tools within the density functional theory (DFT).

The candidates should have experience in the use of quantum chemical programs to carry out *ab initio* electronic structure calculations. Experience in electronic excited state calculations will be highly appreciated. It is required that the candidates have a strong background in theoretical chemistry.

References

- [1] C. Huang, S. Barlow, S. R. Marder. *J. Org. Chem.* 2011, 76, 2386.
- [2] H. Yin, M.-Y. Sui, Q.-Q. Pan, et al. *Dyes Pigments* 2013, 98, 160.
- [3] K. M. Lefler, K. E. Brown, W. A. Salamant et al. *J. Phys. Chem. A* 2013, 117, 10333.
- [4] S. W. Eaton, L. E. Shoer, D. Karlen, et al. *J. Am. Chem. Soc.* 2013, 135, 14701.

- *Electronic correlations and thermal stability in topological materials*

Contact person: Maia Garcia Vergniory (maiagvergniory@dipc.org).

Reference: 2018/36.

Topological insulators, theoretically proposed and swiftly experimentally discovered eleven years ago, have since dominated solid state physics. Along with topological semimetals they caused a paradigm shift in our understanding of phases of matter. Moreover, they display exotic transport properties such as robust surface states or high negative magnetoresistance [1], exhibiting a remarkable symbiosis between elegant mathematical theories, accurate material and technological applications [2].

The state-of-the-art theoretical predictions are based on first principles calculations combined with group symmetry analysis [3,4]. However, this non-interacting ordered picture can only be applied to very low percentage of materials in nature. In this project we will tackle a new research line that is taking off in the field: topological properties and electronic structure in strong correlated electrons. These strong interactions can induce topological transitions and enhance the electronic gap.

During this project we plan to study these interactions by implementing ab initio Density Mean Field Theory as well as develop an interacting group theory to evaluate the symmetries under which the wave function transforms. The new topological phases these correlations can induce will also be studied.

- [1] XL Qi, SC Zhang, Reviews of Modern Physics 83 (4), 1057 (2011)
- [2] BA Bernevig, TL Hughes, SC Zhang, Science 314 (5806), 1757-1761 (2006)
- [3] J. L. Mañes Phys. Rev. B 85, 155118 (2012)
- [4] B. Bradlyn et al., Science 353 , 6299 (2016)