



CALL FOR APPLICATIONS - November 2022

PhD Student Position

Donostia International Physics Center (DIPC) is currently accepting applications for PhD Student positions. This is a unique opportunity for highly motivated students, recently graduated from the university in Physics or related fields, to join one of DIPC's high-profile research teams. A description of each of the available openings, contact information and deadlines can be found on the following pages.

Although candidates are welcome to contact the project supervisors to know further details about the proposed research activity, please be aware that the application will be evaluated only if it is submitted directly to the email address listed as "application email".

Applications received by the deadline will be evaluated by a Committee designed by the DIPC board on the basis of the following criteria:

- CV of the candidate (60%)
- Adequacy of the candidate's scientific background to the project (20%)
- Reference letters (10%)
- Other: 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 may revoke its decision if the candidate fails to join by the appointed time, in which case the position will be awarded to the candidate with the next highest score, provided it is above 50 (out of 100).

However, the selected candidate may keep the position if, in the opinion of the Selection Committee, the candidate duly justifies the reasons why he or she cannot join before the specified deadline, and as long as the project allows it.

Ref. 2022/84
Benchmarking of nonlinear optical properties

Supervisor(s):

*Eduard Matito (ematito@dipc.org)
Josep M. Luis (josepm.luis@udg.edu)*

Duration: 1 year

Application Deadline: 30/11/2022

Application Email: jobs.research@dipc.org

Response properties, especially the high-order ones, are very sensitive to the electronic structure methods and thus represent a long-standing challenge with widespread applications in chemistry, physics, and biology. Response properties refer to changes in the molecule upon the action of an external perturbation. They include excitation energies, linear and nonlinear optical properties (NLOPs), one- and multi-photon transition rates, and multiple spectroscopic magnitudes such as vibrational frequencies.

With the growth of computer power, the calculation of these properties is becoming more standard, unveiling some severe limitations of current electronic structure methods.

The accurate NLOP and vibrational spectra calculation is essential to studying many state-of-art problems such as chemical reactions under external electric fields. The main goal of this position is to surface some limitations of current electronic structure methods and develop new ones tailored for response properties. In particular, we will contribute to developing reliable electron structure methods to calculate NLOPs and vibrational spectroscopies, aiming at these objectives:

- Identify the limitations of electronic structure methods to calculate molecular properties.
- Develop new electronic structure methods that overcome these limitations.

We are looking for candidates with a master's in theoretical chemistry and experience working with quantum chemistry methods. It will be especially considered if the candidate has experience working with linear and nonlinear optical properties.

Interested candidates should submit an updated CV and a brief statement of interest to the application email listed above. Reference letters are welcome but not indispensable. The reference of the specific opening to which the candidate is applying should also be stated in the subject line.