



CALL FOR APPLICATIONS - October 2022

Research Assistant Position

Donostia International Physics Center (DIPC) is currently accepting applications for Research Assistant positions. This is a unique opportunity for highly motivated students, recently graduated from the University in Physics or related fields, to gain research experience in 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. 2022/65

Designing organic molecules for reversible charge-to-spin conversion

Supervisor(s):

Daniel Reta (daniel.reta@ehu.eus)

Duration*: 1 year

Application Deadline: 21/10/2022

Application Email: jobs.research@dipc.org

Organic molecular magnetism is a rapidly evolving field that offers exciting applications in areas ranging from qubits to chemical synthesis. However, the currently available molecular architectures exploit only a fraction of the available chemical space, and consequently, the potential of organic magnetism is somehow constrained. Current efforts in our group aim at remedying this and focus on establishing a general and reversible approach to introduce magnetic properties in broader families of organic molecules. For this, we employ a concerted experimental and computational approach.

Building on ongoing studies at the group, in this project you will use computational chemistry methods to i) characterise diradical formation in a series of biologically active organic molecules and ii) assess the diradical character role in the molecular biological function.

To that end you will employ sophisticated density functional and wavefunction-based electronic structure methods applied to multistate models of increasing complexity: from the isolated molecule, to solvated systems, to protein-molecule complexes. At the latter stage, using reported crystal structures, molecular dynamics will also be employed to describe possible radical-based chemical reactivity between the molecule and nearby protein residues. Across the multiple targeted molecules, structure-property correlations will be drawn to propose clear design strategies and obtain tuneable diradical character.

Your work will be carried out in close contact with results obtained from EPR and magnetometry characterisation techniques. Depending on your preferences, you will also be able to employ spin Hamiltonians to model the experimental magnetic data.

The candidate is expected to have a good knowledge of organic chemistry, quantum mechanics and electronic structure theory of molecules, as well as excellent oral and written communication skills in English.

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.

***Initial funding is for 1 year, renewable to 4 years. Application for external funding via fellowships will be expected and supported.**