



CALL FOR APPLICATIONS - February 2023

Post-doctoral Position

Donostia International Physics Center (DIPC) is currently accepting applications for Post-doctoral positions. This is a unique opportunity for junior researchers with a recent PhD degree 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 (40%)
- Adequacy of the candidate's scientific background to the project (40%)
- 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. 2023/37
Computational study of tunnelling in organic reactions under pressure

Supervisor(s):
Bo Chen (bo.chen@dipc.org)

Duration*: 3 years

Application Deadline: 28/02/2023

Application Email: jobs.research@dipc.org

Quantum mechanical tunnelling is a common phenomenon in organic reactions. Tunnelling probability depends on, among many things, the width of the reaction barrier, the mass of the tunnelling particle, and the energy deficiency of the molecule to reach the top of the barrier. The barrier width is more important than the mass and the energy deficiency in determining the tunnelling probability of a reaction. Most experimental and computational studies on tunnelling are for low pressure (1 atm or lower) reactions.

Tunnelling in high-pressure reactions is rarely investigated, though evidence for tunnelling under pressure has been observed. Pressure can change the shape of the potential energy surface of a reaction (for example, the height and width of the barrier) and the electronic structure of the molecule, so will likely have a significant effect on the tunnelling probability of a reaction. The hypothesis is that compression (high pressure) shortens covalent bonds and intermolecular vdW distances, and favours “crowded” conformations of a molecule, which may lead to narrower barriers for reactions such as intermolecular H-transfer reactions or bond-formation reactions, and intramolecular electrocyclizations and certain isomerizations. If the reduction of barrier width is a general phenomenon under pressure, tunnelling could be more common in high-pressure reactions.

The project will involve the collaboration with Prof. Roberto Cammi at University of Parma, Italy, for developing the essential eXtreme Pressure-Polarizable Continuum Model (XP-PCM) method and for the application of the method to tunnelling under pressure.

Essential:

- PhD in computational chemistry, organic chemistry or related fields
- Proficiency in quantum chemistry software, such as Gaussian
- Proficiency in communication and writing in English
- Motivation; ability and willingness to work in a collaborative, cross-disciplinary research environment.

Preferable:

- Experience with tunnelling calculations, from simple Bell corrections to sophisticated SCT/LCT calculations.
- Experience with high-pressure chemistry and/or physics research
- Experience with Julia and/or Fortran programming language

Interested candidates should send an up-to-date CV, a statement of interest, and 2-3 reference letters. The letters can be arranged to be sent directly by the references. The candidate should explain in the statement how his/her background and/or interest align with the project. The reference of the specific opening to which the candidate is applying should also be stated in the subject line.

This project has received funding from the Spanish Government's grant program "Proyectos de Generación de Conocimiento" under grant number PID2021-123573NA-I00



***Openings with a duration of more than one year are for a 1-year contract, renewable based on performance and availability of funding.**