

JOB OFFERS AT DIPC: QUANTUMCHEMPHYS LABORATORY

The Theoretical Chemistry and Physics at the Quantum Scale ("QuantumChemPhys", <http://www.quantumchemphys.org/>) is a Transborder Joint Laboratory (LTC - Laboratoire Transfrontalier Conjoint) created by the University of Bordeaux (UBx), the University of the Basque Country (UPV/EHU), and the Donostia International Physics Center (DIPC).

The purpose of the QuantumChemPhys lab is to strengthen the scientific collaboration among researchers from Euskadi and Aquitaine through the creation of a transnational institution focusing on the theoretical aspects of chemistry and physics at the quantum scale, i.e. the quantitative description of the motion of electrons and nuclei (and their coupling) in solids, at gas-solid interfaces, as well as in the interaction with light. Such a challenge requires the developments of theoretical methods and numerical simulations within the framework of quantum/classical/semiclassical mechanics.

Within this general framework and with the financial support of the Department of Education of the Basque Government through Euskampus Fundazioa, we are opening three positions for brilliant young researchers that are interested in joining this international research environment. All positions will be co-supervised between a senior researcher at UBx and another senior researcher at DIPC – UPV/EHU. Mobility between Bordeaux and Donostia is expected in the development of the projects. In some cases, the project will be pursued in collaboration with research groups of institutions belonging to the ENLIGHT Alliance (<https://enlight-eu.org/>).

In the following pages, we are listing the profiles currently needed at DIPC and that will be funded through Euskampus Fundazioa. A description of each of the available openings, contact information and deadlines can be found in these pages. Openings with a duration of more than one year are for a 1-year contract, renewable based on performance.

Candidates are welcome and even encouraged to contact the project supervisors to know further details about the proposed research activity. However, please be aware that the application will be evaluated only if it is submitted directly to the email address listed as "jobs.research@dipc.org".

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.

Interested candidates should submit an updated CV and a brief statement of interest to jobs.research@dipc.org before next March 11, 2022. 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.

Ref. 2022/14 – PhD position: Computational study of mechanoluminescence properties of organic materials

Since the concept was first coined 20 years ago, aggregation induced emission (AIE), a photophysical phenomenon in which single molecule emission is enhanced by aggregate formation, has seen a growing interest from the materials science community owing to its vast potential in optical, electronic, energy and biomedical applications. AIE encompasses a variety of research branches, among which mechanoluminescence (ML) constitutes the central phenomenon of this proposal.

Mechano-responsive organic materials belong to the class of so-called “smart” materials and have received ever-increasing attention in the past decade as appealing candidates in a wide range of promising applications, from sensing devices to security inks. While the luminescent properties of individual organic compounds are now well described and controlled by suitable molecular design, their optical response in the solid-state is far from trivial as it is strongly affected by aggregation effects, i.e., molecular packing and associated intermolecular interactions. Under the application of a mechanical force, such as shearing, stretching or crushing, the supramolecular arrangement is altered, and in turn the luminescence properties affected.

The rational development of new improved systems is currently hampered by the complexity of the ML phenomenon, which can originate from different electronic, structural and aggregation effects and translate into fluorescence or phosphorescence (i.e., involving different excited states). So far, no theoretical studies have been carried out to exhaustively assess ML of organic materials, from the individual molecular structure and photophysical properties to their solid-state mechanoluminescent response. In particular, computational investigations can provide insights into the experimentally unknown detailed molecular organization in amorphous phases.

In this context, we aim to combine quantum and classical computational techniques to investigate the structural and electronic origins of ML in organic materials.

The project will be conducted in partnership between DIPC and Univ. Bordeaux as part of the Theoretical Chemistry and Physics at the Quantum Scale (“QuantumChemPhys”) Transborder Joint Laboratory (<http://www.quantumchemphys.org>) activities, and under the co-supervision of Dr. C. Tonnelé (DIPC) and Prof. F. Castet (Univ. Bordeaux).

The candidate should hold a Master in Chemistry, Physics or Physical Chemistry with a background in computational chemistry. A good level in written and spoken English is also required. Programming skills are a plus (Fortran, Python, bash scripting...).



Contact:

- Claire Tonnelé (claire.tonnele@dipc.org)
- Frédéric Castet (frederic.castet@u-bordeaux.fr)

Ref. 2022/15 – Post Doctoral position: Elementary reactive processes of hydrogen at tungsten surfaces in the context of fusion energy developments

Because of their prominent role in phenomena of natural and technological relevance, elementary chemical processes at surfaces have been intensively investigated both experimentally and theoretically for decades. In particular, the interaction of hydrogen isotopes with the tungsten surface is a vivid field of research within the framework of nuclear fusion.

Understanding the microscopic mechanisms responsible for hydrogen trapping/de-trapping from surfaces containing atomic impurities is a current issue. Within this project the dynamics of sticking and desorption of atomic and molecular hydrogen from tungsten surfaces containing oxygen and nitrogen impurities will be investigated.

Such approaches will rely on Density Functional Theory studies, ab initio molecular dynamics, the development of neural networks for the representation of multidimensional potential energy surfaces and quasi-classical molecular dynamics in close connection with experiments.

The project will be conducted in partnership between DIPC and Univ. Bordeaux as part of the Theoretical Chemistry and Physics at the Quantum Scale ("QuantumChemPhys") Transborder Joint Laboratory (<http://www.quantumchemphys.org>) activities, and under the co-supervision of Maite Alducin (CFM and DIPC) and Pascal Larregaray (Université de Bordeaux / CNRS).

Contact:

- Maite Alducin (maite.alducin@ehu.eus)
- Pascal Larregaray (pascal.larregaray@u-bordeaux.fr)

Ref. 2022/16 – Post Doctoral position: Computational design of Baird-aromatic dyes for singlet fission

In the last decade a lot of interest has been put in the development of singlet fission materials as a novel strategy to overcome the Shockley-Queisser limit for single junction photovoltaics. Singlet fission is a photophysical reaction in which one absorbed photon of light is split into two triplet excitons.

This project will employ the excited state aromaticity concept to design new molecular materials for singlet fission. Recently, the group of Prof. Ottosson has described a general strategy for singlet fission chromophore design based on a combination of the ground and excited states aromaticity rules [J. Am. Chem. Soc. 2020, 142, 5602]. Through this qualitative model one can identify new molecules with suitable energy orderings for singlet fission by plotting the state energies against an approximate (anti)aromaticity coordinate.

The present project aims to use quantum chemical calculations to design new classes of compounds suitable as efficient singlet fission chromophores utilising this new design strategy. More specifically, in the first part of the project we will use substituent and (hetero) benzannelation strategies to tune the extent of excited state aromaticity to arrive at compounds tentatively suitable as singlet fission chromophores. Secondly, we will investigate the suitability of the designed chromophores to form singlet fission solid state materials by exploring the electronic structure properties of their aggregation arrangements.

The candidate should have a good knowledge of quantum chemistry and molecular photophysics, and a solid formation in theoretical and computational chemistry. Experience in the computation of electronic transitions in molecular systems with quantum chemistry methods such as TDDFT and/or wave function-based methods is required. Experience with the use of multilevel techniques such as in quantum mechanics/molecular mechanics methods, will be also taken into consideration.

Contact:

- David Casanova (david.casanova@ehu.eus)
- Frédéric Castet (frederic.castet@u-bordeaux.fr)
- Henrik Ottosson (henrik.ottosson@kemi.uu.se), Uppsala Universitet