

Research PhD contract

More than 60 researchers, experts in different fields of the Theoretical and Computational Chemistry, integrate the Institute of Theoretical and Computational Chemistry of the Universitat de Barcelona, IQTCUB. The research activity carried out at the IQTCUB (<https://www.iqtc.ub.edu/en/>) covers methods and computational tools development, application of several techniques of electronic structures and simulation to problems in materials science, the study of reactivity and reaction dynamics in chemical reactions as well as of biological systems and soft-matter.

The IQTCUB is currently accepting applications for a PhD Position from master students who want to join the Applied Computational Chemistry & Molecular Modelling research group (<http://www.ub.edu/rsogroup/>) and to participate into the project "*Applied computational chemistry for CO₂ capture, separation and conversion into light fuels*" under the supervision of [Prof. Ramón Sayós \(r.sayos@ub.edu\)](mailto:r.sayos@ub.edu) and [Dr. Pablo Gamallo \(gamallo@ub.edu\)](mailto:gamallo@ub.edu).

Details

The aim of this project is to investigate: 1) the capture and separation of CO₂ from post-combustion flue gases using several solid adsorbents (e.g., zeolites or metal-organic frameworks (MOFs)) and 2) the CO₂ conversion into valuable chemicals (e.g., syngas, methanol, methane or formic acid) by using heterogeneous catalysis (e.g., supported metal nanoparticles or functionalized MOFs). Several techniques from the theoretical and computational chemistry field will be applied: Density Functional Theory, Molecular Dynamics, Grand Canonical Monte Carlo and kinetic Monte Carlo, among others. Theoretical results will be compared with experimental data provided by external collaborators from both academic and industrial laboratories.

The PhD position is funded by the Spanish Structures of Excellence María de Maeztu (MDM-2017-0767-19-2 FPI contract) within the research line of clean and secure energy.

Requirements

- A highly motivated and independent researcher with a master's degree in Chemistry, Physics, Materials Science or other related topics. Second-year master students may also apply.
- Strong theoretical chemistry and physics background and computer skills.
- Ability to work collaboratively as a part of a research group.
- Good oral and written communication skills in English.

Applications

Firstly, the interested candidates should send a complete CV (including academic B.Sc. and M.Sc. transcripts), a motivation letter and two reference letters to r.sayos@ub.edu with the subject "MDM-2017-0767-19-2_FPI-XXX", substituting XXX by the candidate surname, before 15th October 2019. Secondly, some of these documents and additional data will have to be introduced into the official web application at the *Ministerio de Ciencia, Innovación y Universidades* once the call is opened (last year was in October 9 - 29). An interview will be part of the selection procedure.

Summary of conditions

Contracts: a bridge contract (first months) + 4-year FPI contract.

Expected salaries: bridge contract (to be negotiated) and FPI contract (16.127 € 1st year until 21.599 € last year, following EPIF conditions).

Starting date of the first contract: 1st November 2019.

Please, you can contact me in case of any question (Prof. Ramón Sayós, phone: 93 4034760).