

Nano-Bio Spectroscopy Group and Institute of Theoretical and Computational Chemistry

Description: PhD position.

Duration: 4 years.

Gross salary: approx. 17 k€/year for the first two years, 18.2 k€/year in the third year and 22.8 k€/year in the fourth year.

Working place: San Sebastián (Spain) with some visits to Barcelona (Spain).

Funding: MORECAT project funded by MICIUN (Spain) via a PhD grant of the FPI type.

PhD advisors:

- Dr. Federico Calle-Vallejo (federico.calle@ehu.es), University of the Basque Country.

<https://scholar.google.com/citations?hl=en&user=Ehc5tVAAAAAJ>

- Prof. Stefan Bromley (s.bromley@ub.edu), University of Barcelona.

<https://scholar.google.com/citations?hl=en&user=GRcDA5cAAAAJ>

Context: the MORECAT project will focus on the computational design and evaluation of a new class of hybrid electrocatalysts. The proposed electrocatalyst systems are based on the general concept of combining redox mediators and metals in novel synergistic systems. We will study a selection of important electrocatalytic reactions: the hydrogen oxidation and evolution reactions (HOR/HER), the oxygen reduction reaction (ORR) and CO₂ reduction (CO₂RR), among others.

Project: The research project will be fully computational and carried out at the University of the Basque country. Interaction with experimental partners of the host groups is anticipated. In addition, some research visits to the University of Barcelona are planned. The project will include (but is not restricted to) the optimization of systems by means of DFT calculations, the location of transition states, and thermodynamic and microkinetic modelling of electrocatalytic processes.

Qualifications: Candidates holding a MSc degree should have a solid background in Chemistry, Physics, Chemical Engineering or Materials Science. Knowledge of basic electrochemistry is a plus. Previous experience with the VASP and/or FHI-AIMS codes are highly appreciated. Experience in bash scripting, python and the atomic simulation environment (ASE) is desirable. Excellent communication skills in English (listening, speaking, writing, and reading) are a must. However, candidates need not speak Spanish, Basque or Catalan to apply or carry out their PhD project.

Location: The Nano-Bio spectroscopy group is located at the University of the Basque Country (Korta building, Gipuzkoa campus, San Sebastián). IQTC is located at the University of Barcelona (Barcelona, Spain).

Application: Please send an email application including a 1-page cover letter, a short CV, and the contact details of two referees. Please address your email to federico.calle@ehu.es and write in the subject "MORECAT PhD position".