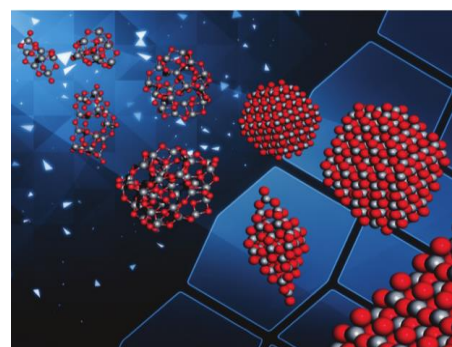


Open FPI PhD position:

“Designing New Photoactive Nanomaterials”

The devastating climatic and environmental effects of burning fossil fuels are now firmly established. Clearly, reliable and renewable sources of more environmentally friendly energy are needed. Hydrogen is alternative clean fuel that can be produced through the sunlight-driven photocatalytic splitting of water. Currently, however, this process is not efficient and new technological advances are needed to enable affordable and sustainable hydrogen production. In this project we will use computational chemistry modelling and machine learning techniques to design and understand new photocatalytic nanomaterials for water splitting. The focus will be on inorganic nanomaterials (e.g. TiO_2 and ZnO nanoparticles) which offer huge potential due to the possibilities of finely tuning their optical, electronic and chemical properties via various means (e.g. size, shape, crystallinity, dimensionality and surface chemistry).

The PhD research will form a core part of a recently government-funded research project: "*Rational design of new heterogeneous, electro- and photocatalysts for sustainable clean energy production via greenhouse gas conversion and hydrogen generation*" and will build on significant recent advances made in our group modelling low-dimensional inorganic nanosystems, such as: ***Understanding the interplay between size, morphology and energy gap in photoactive TiO_2 nanoparticles*** A. Morales, A. Macia-Escatllar, F. Illas, S. T. Bromley, *Nanoscale* (2019) 11, 9032.



The PhD project will be conducted in the Computational Materials Science Laboratory (www.ub.edu/cmsl/) research group which forms a part of the Institute of Theoretical and Computational Chemistry at the University of Barcelona, IQTCUB (www.iqtc.ub.edu/en/). The IQTCUB integrates more than 100 researchers covering fields such as: modelling of materials and bio-systems, the study of reaction dynamics and the development of computational tools. The IQTCUB was recently awarded the *María de Maeztu* prize for research excellence from the Spanish government.

Requirements

- Master's degree in Chemistry, Physics, Materials Science or other related topics (60 ECTS)
- Ability to work collaboratively as a part of a research group.
- Good oral and written communication skills in English.

A strong background in theoretical chemistry/physics and/or computer programming would be beneficial.

Application procedure

Interested candidates should send a complete CV (including undergraduate and Master's grades), a short motivation letter and names of two referees to: s.bromley@ub.edu with the subject "HEPCAT_FPI-XXX", substituting XXX by the candidate surname, before the 30th of September 2019. A phone/Skype interview will be part of the selection procedure. For any enquiries contact: Prof. Stefan Bromley (s.bromley@ub.edu) or Dr. Angel Morales (angel.morales@ub.edu).

Summary of conditions

4-year FPI (Formación de Personal Investigador) PhD grant with provisionally approved funding from the Ministerio de Ciencia, Innovación y Universidades.

Starting date: 1st October 2019 (if formal start date is later a “bridging” contract will be made to hire the successful candidate until the FPI PhD contract starts)

Expected salary: bridge contract (to be negotiated) + PhD contract (16.127 € 1st year - 21.599 € 4th year).