



PhD Student Position in Computational Modelling of Nanomaterials for Catalysis and Energy-Related Applications, University of Barcelona

We are seeking a highly motivated candidate for a fully-funded PhD student position at the Institute of Theoretical and Computational Chemistry of the University of Barcelona, IQTCUB (www.iqtc.ub.edu/en) under the supervision of ICREA Professor Konstantin Neyman (www.icrea.cat/Web/ScientificStaff/Konstantin-M-Neyman-292) and [Dr. Albert Bruix](#). The PhD project is devoted to computational investigation of complex nanostructured inorganic materials using a combination of methods based on quantum mechanics, global optimization algorithms, multiscale modelling and machine learning, building on recent advances of the group.

Requirements

- Either holding a Master's degree (60 ECTS) in Chemistry, Physics, Materials Science (or related fields) or being in position to obtain the degree before the contract starting date. **Therefore, applications from Master's students finishing their degree during the 2020/21 academic year are very welcome.**
- A strong background in theoretical chemistry and/or physics, physical chemistry or related fields. Experience or training in quantum mechanical methods and programming skills is an important advantage.
- High motivation, curiosity and ability to work collaboratively as part of an international research team.
- Good oral and written communication skills in English.

We offer

A 4-year fully-funded PhD position in a vibrant research environment with international collaborations including outstanding experimental partners. The position is funded by the María de Maeztu Excellence Unit Program of the Spanish Ministry of Research, Innovation and Universities (through a *Formación de Personal Investigador* PhD grant). A bridging contract could be negotiated for the period from the application date for the FPI grant until the official start of the employment anticipated for the summer 2021.

Application procedure

Qualified candidates should send a motivation letter, Curriculum Vitae (including undergraduate and Master's grades) and contact details of two referees per e-mail to Dr. Albert Bruix [abruix\(at\)ub.edu](mailto:abruix(at)ub.edu) before **September 30, 2020**. An online interview will be part of the selection procedure. Short-listed candidates will be contacted and asked to apply formally through the application website of the Spanish Ministry of Research, Innovation and Universities.