Institut de Química Teòrica i Computacional
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU

PhD position in Computational Chemistry, Barcelona, Spain

Modelling Nanomaterials for Catalysis and New Energy Technologies

The Institute of Theoretical and Computational Chemistry of the University of Barcelona, IQTCUB (www.iqtc.ub.edu/en/), is seeking for a PhD candidate to work in the area of computational materials science and catalysis. The position is offered in the group *Reactivity of Nanostructures* led by ICREA Professor Konstantin Neyman (www.icrea.cat/Web/ScientificStaff/Konstantin-M-Neyman-292 and will be co-supervised by Dr. Albert Bruix.

The PhD study is part of a research project PGC2018-093863-B-C22 funded by the Spanish Ministry of Research, Innovations and Universities and built on significant recent advances the group has made in modelling inorganic nanomaterials, for instance:

- The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. *Nature Materials* 17 (2018) 519
- Counting electrons on supported nanoparticles. *Nature Materials* 15 (2016) 284
- How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. *Chemical Science* 6 (2015) 3868

Requirements

- Master's degree in Chemistry, Physics, Materials Science or a related field (60 ECTS)
- A strong background in physical and theoretical chemistry/physics paired with high motivation and curiosity
- Ability to work collaboratively as part of an international research team
- Good oral and written communication skills in English

Application procedure

Interested candidates should send a motivation letter, CV (including undergraduate and Master's grades) and names and contact details of two referees per e-mail to Dr. Albert Bruix (albert.bruix(at)ch.tum.de) before **October 31, 2019**. A phone/Skype interview will be part of the selection procedure. Only short-listed candidates will be contacted, and asked to apply formally through the application website before the deadline November 7th, 2019.

We offer

A 4-year PhD position funded by the Spanish Ministry of Research, Innovation and Universities (through a *Formación de Personal Investigador* PhD grant. The starting employment date is spring 2020. If necessary, a bridging contract could be negotiated for up to six month before the official start of the FPI grant.

2019/10/15