

## **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/](http://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  
<http://www.icrea.cat/Web/ScientificStaff/Konstantin-M-Neyman-292>

The PhD study is a 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 made in modelling inorganic nanocomposites, 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 a part of an international research team
- Good oral and written communication skills in English

#### **Application procedure**

Interested candidate should send a motivation letter, CV (including undergraduate and Master's grades) and names of two referees per e-mail to Prof. Konstantin Neyman ([konstantin.neyman@icrea.cat](mailto:konstantin.neyman@icrea.cat)) before October 31, 2019. A phone/Skype interview will be part of the selection procedure. Only short-listed candidates will be contacted.

#### **We offer**

An FPI (Formación de Personal Investigador) PhD grant for up to 4 years with provisionally approved funding from the Spanish Ministry of Research, Innovations and Universities. A call to apply for the FPI grant will be opened on October 17, 2019 with the application deadline November 7, 2019. A starting employment date of a successful candidate is expected to be in the spring 2020. If necessary, a bridging contract could be negotiated for up to six month before the official start of the FPI grant.