

Open PhD position

Understanding Mixed Metal-Oxide Nanosystems

Highly qualified students with an interest in nanoscience and computational chemistry are invited to send their application for an open PhD position.

Project

Nanostructures and nanostructured materials based upon intimately mixing oxide materials have drawn much recent attention due to their huge potential for applications in a diverse range of important fields including gas sensing, (photo)catalysis, photonics/optical devices (e.g. wave guides, solar cells), tailored multi-(bio)functional supports and self-cleaning coatings. These novel properties often emerge from the unique and complex manner in which oxide materials combine at the nanoscale. Although some macroscopic oxide alloys and composites are well studied, mixed metal-oxide nanosystems are generally little understood from a fundamental perspective. Starting with the important prototypical $\text{TiO}_2\text{-SiO}_2$ semiconductor-insulator system, the candidate will use computational modelling to systematically explore how these oxides combine at the nanoscale. Throughout this investigation the structure and properties (e.g. energetic stability, reactivity) will be assessed. Based upon results obtained, other mixed metal-oxide nanosystems will be chosen and similarly investigated. The information gained will be used to get an overall perspective of how oxides mix at the nanoscale and to predict new systems for applications (e.g. catalysis, nanostructured materials).

Several computational modelling techniques (e.g. density functional theory, *ab initio*/classical molecular dynamics, global optimisation) will be employed during the project to achieve the objective.

Overview

The thesis will be co-supervised by Prof. Stefan Bromley at the University of Barcelona in Spain and Prof. Monica Calatayud at the University Pierre and Marie Curie, in Paris, France, as a part of the Innovative Training Networks of the Marie Skłodowska-Curie Action **ITN-EJD-642294. TCCM ESR11**. The PhD will split between Paris (20 months) and Barcelona (16 months) with a 2 month secondment at Simune. Upon completion of the thesis the title of doctor will be awarded by both universities.

Salary: 3000 €/month gross salary (plus expenses for inter-laboratory travel and conferences).

Duration: 3 years

Deadline for applications: April 15th (for starting before end of September 2015)

Requirements

- The candidate should have a strong background in physical chemistry and a Masters degree in a relevant discipline.
- Experience in computational chemistry techniques and/or programming would be appreciated.
- At the time of recruitment the candidate must not have resided or carried out their main activity (work, studies, etc) for more than 12 months in France or Spain in the immediately preceding 3 years.

Contact

Candidates should submit a Curriculum Vitae and a motivation letter to:

s.bromley@ub.edu and calatayu@lct.jussieu.fr

Official application must be submitted via the website: http://emtccm.qui.uam.es/?page_id=1282