



PhD in Computational Modelling of Novel Catalysts for Sustainable Energy Applications (Starting Date: September 2017)

Applications are invited for a 4-year PhD scholarship (16,000€/year + fees covered) in Computational Modelling of Novel Catalysts for Sustainable Energy Applications in the research group of Dr. Max García-Melchor at Trinity College Dublin (TCD). Dr. García-Melchor is an Assistant Professor in Chemical Energy Systems based in the School of Chemistry of TCD and with a very strong track record and international reputation in the theoretical description of homogeneous and heterogeneous catalytic processes. His research group has been recently established at TCD with a vision for developing a strongly performing international team in this field.

Project

The project will involve the use of state-of-the-art density functional theory methods to reach a fundamental understanding of catalytic systems for renewable energy applications, and the use of this knowledge to rationally design novel materials with a predicted superior performance. The successful candidate will be directly supervised by Dr. García-Melchor and will receive training in the modelling of chemical reactions catalysed by molecular complexes and solid surfaces. The candidate will also be instructed in the use of supercomputers based at the Trinity Centre for High Performance Computing (TCHPC) and the Irish Centre of High-End Computing (ICHEC), which the group of Prof. García-Melchor has access to.

Responsibilities and Conditions

The successful candidate will join an exciting and dynamic research team and will be encouraged to develop his/her chemical knowledge, and technical and transferable skills. The candidate will attend courses on the Dublin Chemistry programme, group meetings, seminars, as well as international conferences. This scholarship will allow the candidate to develop advanced computational chemistry skills and gain particular expertise in the modelling of (electro)chemical processes involving molecular and solid catalysts. On graduation the candidate should be well placed to pursue a career in either the materials science industry or as an academic researcher.

Eligibility Criteria

Applications are welcome from strongly motivated candidates with, or expecting to gain, a first or upper second class honours (or equivalent) Bachelor/Master degree in Chemistry, Computational Chemistry, Nanotechnology, or related discipline. Previous experience in molecular modelling and programming will be a plus. Good oral and written communication skills in English are required.

Application Process

Applications must include a cover letter, CV (resume), and the contact details of at least 2 referees. Documents should be emailed to Dr. García-Melchor (garciamm@tcd.ie) by June 21st 2017 at 17:00 Dublin local time. Shortlisted candidates may be interviewed at TCD or remotely via Skype. All candidates will be notified of the application outcome in due course. For further information, see: <http://www.chemistry.tcd.ie/staff/academic/garciamm/>
https://www.tcd.ie/Graduate_Studies/students/prospective/apply/