



**Trinity College Dublin**

Coláiste na Tríonóide, Baile Átha Cliath

The University of Dublin

## PhD studentship in Computational Materials Chemistry & Electrocatalysis

Applications are encouraged for a fully funded 4-year PhD position in the Computational Catalysis and Energy Materials group ([www.ccem-group.com](http://www.ccem-group.com); [@CCEM\\_Group](https://twitter.com/CCEM_Group)) led by Prof. Max García-Melchor ([@MGarcia\\_Melchor](https://twitter.com/MGarcia_Melchor)).

Electricity from renewable sources can be used to reduce the carbon footprint and energy intensity of reactions which are important in our economy. However, novel electrode materials need to be developed to enable this transition towards greener industrial syntheses. This project aims to combine quantum chemical methods and artificial intelligence to rationally design highly efficient electrocatalysts to promote novel organic transformations with applications to green hydrogen generation and valorization of bio-resources. The student will develop skills in the areas of computational modelling, electrocatalysis, and machine learning.

The work will be carried out in the highly international and collaborative scientific environment offered by the School of Chemistry at Trinity College Dublin (<https://chemistry.tcd.ie>). This PhD project is funded by [Science Foundation Ireland](https://www.sciencefoundationireland.com) and is part of an inter-university partnership among [Prof. Max Garcia-Melchor](https://www.tcd.ie/chemistry/people/prof_max_garcia_melchor) (TCD), [Prof. Paula Colavita](https://www.tcd.ie/chemistry/people/prof_paula_colavita) (TCD) and [Prof. Suresh Pillai](https://www.atu.ie/chemistry/people/prof_suresh_pillai) (ATU), bringing together expertise in nanomaterials synthesis, fundamental (spectro)electrochemistry and computational chemistry. Therefore, this studentship offers excellent opportunities for developing a strong research portfolio and an interdisciplinary background.

Ideal candidates will be highly motivated, enthusiastic about research, and be in possession of a BSc or equivalent (minimum) in Chemistry, Physics, Computational Chemistry, Nanoscience, Chemical Engineering, or related discipline. Good oral/written communication skills in English are required. Previous experience in molecular modelling and programming is highly desirable. Funding is for 4 years and includes competitive stipend + academic fees at EU-fee level.

**Application deadline: 29 February 2024**

**Starting date: March 2024, or shortly thereafter**

Interested applicants should email their cover letter, CV, academic transcripts, and 2 referee contacts to Prof. García-Melchor at [garciamm@tcd.ie](mailto:garciamm@tcd.ie).