

Doctoral (PhD) position - Iron-sulfur-carbide clusters as models of the nitrogenase active site

Project overview

The accelerating effects of climate change, as well as the economic uncertainty and national security issues associated with dependence on foreign oil and gas for energy, further motivate the development of new and improved alternative energy solutions. Looking to nature for inspiration, the nitrogenase enzyme is a fascinating biological system that has demonstrated the ability to produce ammonia (fertilizer) from air, as well as liquid fuels (petrol) from carbon monoxide, a toxic gas. Thus nitrogenase is capable of producing valuable chemical fuels under ambient conditions, in contrast to industrial processes that require very high temperatures and pressures, which in turn consumes large amounts of energy. The heart of nitrogenase, the site where these chemical fuels are produced, contains an iron-carbon cluster that is unique within biology. To date, synthetic chemists have been unable to reproduce nitrogenase's iron-carbon cluster, limiting our understanding of this complex biological system and how it so efficiently produces valuable chemical fuels.

This research project will develop new technologies to synthesize metal-carbon complexes and materials inspired by nitrogenase and other industrial catalysts. The synthesized complexes will be explored for potential applications to energy storage/conversion and catalysis, as well as fundamental studies on metal-carbide bonding interactions. In particular, the electronic structure and associated chemical reactivities will be extensively explored using advanced spectroscopic techniques, including Mossbauer, Electron Paramagnetic Resonance (EPR), and X-ray absorption and emission spectroscopies. Additionally, spectroscopic studies will be complemented with computational (DFT) analysis.

The position

We are looking for a motivated and inquisitive candidate who is passionate about alternative energy and inorganic synthesis to join our growing research group. The candidate is expected to have a minimum of 2:1H result in BSc (Hons) degree in Chemistry, or equivalent, and meet the [UCD minimum English language requirements](#). This PhD project will focus on the synthesis of iron-sulfur-carbide complexes as models of the nitrogenase active site, as well as their spectroscopic and computational investigations. The ideal candidate will have a solid foundation of synthetic training (organic/inorganic) and familiarity with glovebox and/or schlenk technique. Experience with spectroscopic methods (in particular Mossbauer, EPR, or X-ray spectroscopy) and/or computational (DFT) analysis will be an advantage. The advertised PhD position will be based in the vibrant and expanding UCD School of Chemistry, located in the O'Brien Centre for Science and home to over 100 PhD students.

The location

Ireland's largest university, University College Dublin (www.ucd.ie), is ranked within the top 1% of higher education institutions worldwide. The university is located on a 330-acre parkland campus in the south Dublin suburbs (with three lakes!). Dublin is a lively European capital renowned for its nightlife and bustling technology industry.

The application

Please email a cover letter and CV (including contact information for 2 academic references) to Dr. Justin Henthorn (justin.henthorn@ucd.ie). Applications will be considered on a rolling basis. The position will be filled once the suitable candidate has been identified, therefore early applications are advised. The successful applicant will start in September 2024.

UCD supports equal opportunities and does not discriminate against individuals on the basis of gender, age, race, colour, nationality, ethnic or national origin, religion, marital status, family status, sexual orientation, disability or membership of the traveller community.

Summary

Fully funded PhD scholarship will be awarded for a maximum of 4 years and will include:

- A tax-free stipend of €22,000 per year plus fees for EU students
- Funds for equipment (laptop), travel (international conferences, workshops), and consumables
- Minimum English requirements, see [here](#).

Funding Notes

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