

## **Project Overview**

A joint computational/experimental PhD position (4 years) is available in the School of Chemistry at University College Dublin in the groups of Dr. Nadia Elghobashi-Meinhardt and Dr. Justin Henthorn. The position lies at the intersection of computational biophysics and metallocatalysis, with a focus on novel catalytic centers that are inspired by nitrogenase, the only enzyme in Nature capable of reducing molecular nitrogen. This interdisciplinary project will leverage computational modeling and experimental synthesis and spectroscopic methods to engineer novel FeS carbide compounds.

## **Tasks**

The successful candidate will be involved in: 1) Constructing models and carrying out high-level quantum mechanics/molecular mechanics (QM/MM) computational studies to predict the structures and stabilities of novel carbide structures; 2) Synthesizing and characterizing carbide materials, integrating experimental results with computational predictions; 3) Developing new experimental methods and procedures to improve the synthesis of carbide materials; 4) Characterizing compounds using a range of spectroscopic methods (Mössbauer, EPR, IR, X-ray Absorption/Emission).

## **Candidate Profile**

We are looking for a highly motivated and ambitious candidate with the following qualifications:

- Master's degree (or equivalent) in Materials Science, Physics, Chemistry, or a related field.
- Strong background in computational methods (e.g., DFT, molecular dynamics, or similar) and/or experimental materials synthesis.
- Familiarity with materials characterization techniques such as Mössbauer, EPR, IR, X-ray Absorption/Emission.
- Strong analytical and problem-solving skills.
- Excellent communication and teamwork abilities, with a willingness to work in an interdisciplinary research environment, attend international conferences, and contribute to high-impact journals.

## **Location**

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. Ireland's largest university, University College Dublin ([www.ucd.ie](http://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.

## **How to Apply**

Interested candidates should submit a cover letter, CV, transcripts and certificates of your academic qualifications, and the contact information for two academic or professional references. Please send applications to: [nadia.elghobashi-meinhardt@ucd.ie](mailto:nadia.elghobashi-meinhardt@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. Only applicants who have been selected for an interview will be contacted. The successful applicant will start in September 2025.

For more information about the position, please contact Prof. Nadia Elghobashi-Meinhardt at [nadia.elghobashi-meinhardt@ucd.ie](mailto:nadia.elghobashi-meinhardt@ucd.ie)

We are committed to promoting diversity and inclusion in our research environment and encourage applications from all qualified candidates regardless of gender, age, ethnicity, or background.

### **Summary**

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

- A tax-free stipend of €25,000 per year
- Funds for equipment (computer) and consumables
- Minimum English requirements, see [here](#).

### **Funding Notes**

Funded by a UCD School of Chemistry Sir Walter Hartley Scholarship.