Postdoctoral Researcher in Computational Materials Design for Hydrogen Storage

The Computational Chemistry Group at Trinity College Dublin (TCD), led by Prof. Graeme Watson, is seeking a highly motivated postdoctoral researcher with expertise in (electro)catalytic processes and periodic density functional theory (DFT).

The successful candidate will contribute to the computational modelling and design of materials for green hydrogen production and the valorisation of organic substrates, as part of the EU-funded project PeCATHS (https://pecaths.eu). This interdisciplinary consortium includes leading academic and industrial partners: University Jaume I, CIC energiGUNE, ICN2-CERCA, University of Zurich, Comet Global Innovation, and the European Innovation Marketplace.

Key Responsibilities

- Collaborate closely with computational and experimental partners across the consortium.
- Contribute to research planning, execution, and dissemination through presentations and publications at internal meetings, project reviews, and international conferences.
- Train and co-supervise postgraduate students within the group.

Research Focus

The postdoctoral researcher will be involved in the following tasks:

- Modelling resting states of photo- and electrocatalysts under experimentally relevant conditions.
- Mechanistic investigations of biomass conversion routes to produce liquid organic hydrogen carriers (LOHCs).
- Computational screening and optimisation of catalyst materials to enhance performance and stability.

This role will involve significant collaboration with CIC energiGUNE, with frequent discussion and joint efforts as part of a distributed computational team.

Candidate Profile

Essential Qualifications

- PhD in computational materials science, theoretical chemistry, or a related discipline.
- Strong experience in periodic DFT calculations.
- Excellent written and oral communication skills in English.
- Ability to work both independently and collaboratively in a research team.

Desirable Experience

- Background in modelling (electro)catalytic processes and/or hydrogen storage materials.
- Experience contributing to multi-partner research projects or international collaborations.

Appointment Details

- Start date: 1st September 2025 (or soon as possible thereafter)
- Salary: €44,347 per annum (Point 1 of the IUA Postdoctoral Researcher Scale), with annual increments.
- Contract duration: 18 months, with the possibility of a 12-month extension based on performance and project needs.

Application Process

Interested candidates should send the following documents to Prof. Graeme Watson at watsong@tcd.ie:

- Cover letter outlining their motivation and suitability for the role.
- A full Curriculum Vitae (CV).
- Contact details for two referees.

Informal enquiries are also welcome and can be directed to Prof. Watson at the above email address.