Two 4-year PhD Positions in Computational Quantum Materials Research

Are you interested in using state-of-the-art computational methods to design next-generation quantum materials at the atomic scale? Applications are invited for two fully funded 4-year PhD positions in the School of Physics at University College Dublin (UCD), within the Computational Materials Research group led by Asst. Prof. Nuala Caffrey.

The positions are funded through the Research Ireland Frontiers for the Future project *Quantum Lego*. The project explores how atomically thin two-dimensional (2D) materials can be stacked like LEGO blocks into heterostructures with tailored electronic, magnetic, and structural properties. By integrating first-principles electronic structure calculations, atomistic modelling, high-performance computing, and machine-learning-assisted materials modelling, the project aims to design dynamically tunable quantum materials.

PhD 1: Electrically Tunable Molecular Systems
This project will explore how a switchable electric polarization can be used to control and tune 2D interfaces, with applications in future electronic and spintronic technologies.

PhD 2: Magnetism & Spin-Dependent Phenomena
This project will focus on magnetic interactions in hybrid 2D material systems and how interfacial coupling can be used to engineer emergent properties relevant to quantum materials design.

The successful candidates will join the collaborative Quantum Theory research environment (see www.ucd.ie/quantum) within the UCD School of Physics.

Applicants must:

- Qualify for EU fee status under UCD regulations (see UCD EU Fee Assessment)
- Hold a 4-year Bachelor's degree, or a 3-year Bachelor's degree plus Master's degree, in Physics or a related discipline
- Meet the university's English language requirements (see UCD English Language Requirements)

Experience with scientific programming (e.g. Python, C, or similar) is essential. Previous experience with electronic structure theory, atomistic simulation, machine learning, or high-performance computing is desirable, but not required.

Stipend: €25,000 per year (net); fees covered for students qualifying for EU fee status

Research Budget: Travel support (€1,500/year) and equipment budget (€5,000 total)

Applications should be submitted as a **single PDF file** to **nuala.caffrey@ucd.ie** and should include:

- Academic CV
- One-page statement describing research interests and motivation
- Contact details for two academic referees

Application Deadline: 21st June 2026

Short-listed candidates will be interviewed in early July 2026, with successful candidates expected to begin in September 2026.

Informal Enquiries are welcome and should be directed to nuala.caffrey@ucd.ie