Maynooth University

Ollscoill Mhá Nuad

Department of Chemistry

Details of the Scholarship Award

The Department of Chemistry at Maynooth University is pleased to announce that a PhD Scholarships will be available for suitably qualified and successful applicants intending to commence their PhD studies in September 2026.

We are recruiting up to three PhD researchers as part of a Research Ireland Pathways–funded project based in the Department of Chemistry. The PhD researchers will work on the development and design of advanced polymer–hybrid anion-exchange membranes for electrochemical energy applications. The project brings together computational modelling at multiple length scales, data-driven materials design, and experimental validation to develop membrane materials with improved performance and stability. The research spans computational chemistry, materials science, polymer physics, and electrochemistry, with close interaction between modelling and experimental partners. PhD researchers will be part of a collaborative research team and will contribute to peer-reviewed publications and conference presentations.

PhD Position 1 – Molecular-Scale Modelling

This PhD position focuses on molecular-scale computational modelling of polymer-hybrid anion-exchange membranes. The project involves DFT, molecular dynamics, and Monte Carlo simulations to study ion transport mechanisms, interfacial chemistry, and membrane stability. The researcher will develop structure–property relationships and work closely with experimental partners to validate modelling predictions. Experience or a strong interest in scientific programming and machine-learning-assisted data analysis for materials modelling is an advantage.

PhD Position 2 – Coarse-Grained and Mesoscale Modelling

This PhD position focuses on coarse-grained and mesoscale modelling of polymer-hybrid anion-exchange membranes to understand morphology, phase behaviour, and transport pathways. The project includes developing coarse-grained models, analysing membrane structure–performance relationships, and integrating simulation results with experimental observations. Experience or a strong interest in polymer or soft-matter modelling, scientific programming, and machine-learning-supported optimisation is an advantage.

PhD Position 3 – Computational–Experimental Integration

This PhD position focuses on integrating computational modelling with experimental validation for the development of polymer-hybrid anion-exchange membranes. The project involves translating modelling insights into membrane fabrication strategies, supporting experimental characterisation and electrochemical testing in collaboration with project partners, and feeding experimental results back into modelling and machine-learning-assisted optimisation workflows. A background or strong interest in materials science, electrochemistry, or membrane characterisation, combined with computational or data-driven skills, is an advantage.

Value of PhD Scholarship Award

The awards are fully funded under the Research Ireland Pathways programme for four years. The following funding is available for the successful applicant:

- Student stipend: €25,000 per annum.
- Annual Tuition Fees Support.
- Contribution to Research/ Travel Costs.

Duration of PhD Scholarship Award

The scholarship is awarded for four years of full-time study, subject to satisfactory annual academic progression and continued compliance with Research Ireland funding terms and conditions and institutional regulations.

Role of the student

The PhD student will work under the supervision of Dr Sousa Javannikkhah in the Multiscale Materials Modelling Group. The PhD student appointed to the third position will be co-supervised by Prof. Carmel Breslin. The project is organised around a set of interrelated research tasks focused on the multiscale design and optimisation of polymer–hybrid anion-exchange membranes, combining computational modelling, data-driven analysis, and experimental validation.

The PhD duties will include:

- Working under the supervision of Dr Sousa Javannikkhah, with additional input from project collaborators and experimental partners.
- Developing and applying computational models at different length scales (molecular-scale, coarse-grained, or mesoscale, depending on the specific PhD project).
- Performing simulation-based analysis of membrane structure, ion transport behaviour, and stability, and establishing structure–property relationships.
- Developing and maintaining scientific code and reproducible workflows for simulation, data analysis, and visualisation.
- Applying data-driven and machine-learning-assisted approaches to analyse modelling and experimental data, where appropriate.
- Collaborating with experimental partners to support model validation, interpretation of experimental results, and feedback into membrane design.
- Documenting research outcomes through high-quality scientific writing and contributing to peer-reviewed publications and conference presentations.

- Participating in project meetings, research training, and professional development activities in line with the Research Ireland Pathways programme.

Mode of Study

Awardees must be resident in Ireland and available to pursue their programme of research on a full-time basis at Maynooth University for four years (full-time PhD).

The successful candidate's research programme will be under the general supervision of their nominated supervisor(s) who will specify study times, research times, vacation periods and other operational requirements.

Awardees will normally be based at the Maynooth University campus and may only conduct research elsewhere with the permission of their supervisor and the Head of Department.

Eligibility Criteria for Applicants

Essential Criteria

Applicants must:

- Hold a Bachelor's or Master's degree in, Chemistry, Physics, Materials Science/Engineering, Computational Chemistry, Chemical Engineering, or a closely related discipline.
- Have achieved a First Class or high Second Class Honours (2.1) degree (or equivalent) in their primary degree.
- Demonstrate a strong background in computational and/or experimental materials science, chemistry, or physics.
- Have experience with, or a strong aptitude for, scientific programming and numerical data analysis.
- Demonstrate the ability to work independently and as part of a multidisciplinary research team.

Desirable Criteria

It is desirable that applicants have:

- Prior experience with computational modelling methods (e.g. DFT, molecular dynamics, Monte Carlo, or coarse-grained simulations).
- Experience or strong interest in data-driven or machine-learning approaches for materials science.
- Experience using scientific simulation software (e.g. VASP, CP2K, Quantum ESPRESSO, Gaussian, LAMMPS, DL_MESO, or similar).
- Evidence of research output (e.g. thesis, reports, publications, or conference presentations).
- Good written and oral communication skills in English.

Application and Selection Process

To apply, please submit the following:

- A personal statement describing your academic background, research interests, and motivation for applying to this PhD project.
- A curriculum vitae (CV) outlining your education, research experience, technical skills, and any publications or research outputs.
- A short research proposal (up to 1000 words) explaining your research interests, relevant methods, and how your experience aligns with the project.
- Final academic transcripts for all completed degrees.
- The names and contact details of two referees who can comment on your academic ability and research potential.

Applications will be assessed through an open and competitive selection process. Shortlisting will be based on academic performance, research potential, and the relevance of previous experience to the project. Shortlisted candidates may be invited to interview.

Applicants whose first language is not English are required to provide evidence of English language proficiency in line with the programme-specific requirements of the Maynooth University International Office.

Please note that all scholarship awards are subject to approval for registration by Maynooth University and compliance with Research Ireland Pathways and Maynooth University policies and regulations.

Informal queries can be sent to sousa.javannikkhah@mu.ie

All eligible candidates will be considered for open positions. Applicants may be shortlisted for interview and, if so, will be contacted directly by the Department. Late applications will not be considered.

Please submit completed applications directly to: sousa.javannikkhah@mu.ie.

Closing Date: Please apply by 5pm on Friday 20 March 2026

HR EXCELLENCE IN RESEARCH

Taighde Éireann
Research Ireland