

PhD Studentship in Multi-Scale Electrochemical Modeling:

Position Overview:

One doctoral (PhD) position (4 years) is available to work in the Community of Researchers Assessing Chemical Transformations and Exploring Reactivity (CoReACTER) within the School of Chemistry at University College Dublin. The doctoral student will be supervised by Dr. Evan Walter Clark Spotte-Smith, an Assistant Professor in the School of Chemistry. This position is intended to begin September 1, 2026.

The aim of this project is to develop a fundamental understanding of cross-talk reaction mechanisms in electrochemical systems, with a primary focus on Li-ion and Na-ion batteries. Cross-talk occurs when reductive products formed at the battery's negative electrode transport to the positive electrode and/or oxidative products formed at the battery's positive electrode transport to the negative electrode via some combination of diffusion, migration, and convection. Once at the opposite electrode, these products engage in further reactivity, frequently hampering electrochemical performance. Although cross-talk is recognized as an important process in many electrochemical systems, including metal-ion batteries, little is known about cross-talk mechanisms.

In this project, the student will use multi-scale modeling, combining elementary reaction mechanisms with mesoscale and continuum-scale multiphysics simulations to study the time evolution of battery electrolytes and interphases. This project will involve developing multi-scale simulation methods, but technical aims related to mitigating electrolyte degradation and improving battery stability are also important. Extensions to electrochemical systems beyond metal-ion batteries (e.g., electrocatalysis, electro-organic synthesis) are possible. Note that this is a purely computational and theoretical position, with no laboratory or experimental component.

One scholarship of stipend €25,000 per annum is available for 4 years for the successful applicant. Fees will be also covered. There will be a requirement to teach in undergraduate laboratories and tutorials as part of the scholarship.

Tasks:

The successful candidate will be involved in:

1. Applying first-principles and machine learning-based atomistic simulations to predict (electro)chemical reaction pathways
2. Designing and implementing multi-scale electrochemical simulations combining elementary reaction mechanisms with multi-phase mesoscale and/or continuum-scale simulations
3. Contributing to and maintaining open-source software packages related to reaction pathway analysis, mesoscale and/or continuum-scale modeling, and automated simulation and analysis workflows
4. Developing a detailed mechanistic understanding of the interactions between oxidative and reductive processes in metal-ion batteries
5. Communicating scientific findings publicly through formal (e.g., preprints, journal articles, conference posters, and presentations) and informal avenues

Desired Qualifications:

We are looking for candidates who:

- Hold a Bachelor's (required) or Master's (preferred) degree in chemistry, chemical engineering, materials science and engineering, or a related field;
- Emphasize teamwork, collaboration, and building positive community;

- Have experience in software development/engineering in at least one general-purpose programming language (e.g., Python, Julia, C/C++, Fortran, Rust). Experience with scientific, numerical, and/or GPU programming is a plus;
- Have prior experience with electrochemistry and/or energy storage devices;
- Have skills or experience related to chemical thermodynamics, kinetics, and (especially mass and charge) transport;
- Are familiar with chemical simulation techniques, including but not limited to density functional theory, molecular dynamics, (kinetic) Monte Carlo modeling, finite-element modeling, and multi-scale or multiphysics simulations;
- Hold values such as honesty, modesty, collectivism, justice, kindness, and curiosity and are committed to the ethical practice of science;
- Have skills in (scientific) written and oral communication and want to apply these skills to share research findings;

Candidates who do not meet all of these criteria should not feel discouraged. If you are interested in the project and committed to learning and growth, please feel free to apply.

How to Apply:

Interested candidates should submit a brief (1 page or less) cover letter, CV, academic transcripts, and certificates of your academic qualifications to evan.spotte-smith@ucd.ie or to CoReACTER@proton.me. In your cover letter, please be sure to address the following:

- Why are you interested in working on this project?
- Why, specifically, are you interested in working with (and within) the CoReACTER?
- What is your dream vacation destination?

For more information about the position, please contact Dr. Spotte-Smith at evan.spotte-smith@ucd.ie. For more information about the CoReACTER, including our philosophy and research interests, please see <https://CoReACTER.org>.

We are committed to promoting equity, diversity, inclusion, and belonging in the CoReACTER. We encourage applications from candidates of all backgrounds and especially encourage candidates from marginalized backgrounds (along dimensions such as gender, disability, madness, sexuality, age, ethnicity, race, family status, socioeconomic status, Roma/Traveller status, nationality, and religion, as well as intersections thereof) to apply.