Funded PhD with Assistant Professor Evan Spotte-Smith, UCD School of Chemistry

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 Spotte-Smith, an Assistant Professor in the School of Chemistry. This position is intended to begin January 1, 2026.

The aim of this project is to develop and apply computational methods for statistical learning on chemical reaction network (CRNs) structures. Of particular interests are (directed) hypergraph neural networks, which can be used to predict vertex (molecule), hyperedge (reaction), or hypergraph (network) features. While this project will be heavily focused on algorithm design and software development, especially in its early stages, we also intend to employ the methods developed for such applications as electrolyte decomposition in metal-ion batteries or biomass pyrolysis.

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. Devising and implementing algorithms for machine learning (ML) on hypergraphs generally and CRNs specifically and contributing to related open-source codebases

2. Constructing and disseminating CRN datasets from the prior literature and from atomistic simulations to be used in training, testing, and evaluating CRN ML models

3. Designing and developing CRN ML architectures for tasks of chemical interest, including reaction property prediction and reaction link prediction.

4. Predicting the properties and outcomes of complex reactive processes (e.g., electrolyte decomposition, biomass pyrolysis) via a combination of atomistic simulations and CRN ML

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++, Go, Fortran, Rust). Experience in Julia is a plus, as is experience with scientific, numerical, and/or GPU programming;

- Have some prior experience with data science and/or machine learning;

- Hold values such as honesty, modesty, collectivism, justice, kindness, and curiosity and are committed to the ethical practice of science;

- Are familiar with atomistic simulation techniques, including but not limited to density functional theory and molecular dynamics;

- Have skills in (scientific) written and oral communication and want to apply these skills to share research findings in scientific meetings/conferences and journals; and

- (Preferably) have some exposure to (hyper)graph theory, network science, and/or reaction mechanism/CRN studies.

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 least favorite word (in any language), and why?

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