THE UNIVERSITY of EDINBURGH
School of Chemistry

Data-driven Catalyst Optimization for CO_2 Utilization Reactions

A PhD studentship is available in the groups of Dr Ephrath Solel Moroshko and Dr Antonia Mey (University of Edinburgh; School of Chemistry).

The studentship is fully funded for 48 months by the University of Edinburgh and covers tuition fees and an annual stipend at the UKRI rate (for 2025-26 this is £20,780 per annum). The entry and eligibility criteria can be found at: Entry and Eligibility criteria | E5 Doctoral Training Partnership | E5 Doctoral Training Partnership

Project Summary:

Using computational chemistry and machine learning methods, this project will study the mechanism of CO_2 epoxidation reactions and build reactivity-predicting models, which will be used to design novel highly-efficient catalysts.

CO_2 is one of the most significant contributors to global warming, emitted in large amounts from fossil fuel combustion, industrial processes, and land-use changes. With climate change posing an existential threat, innovative solutions are needed to reduce CO_2 emissions. Among the most promising strategies for this is carbon capture and utilization (CCU), where CO_2 is repurposed into valuable chemicals rather than being treated as waste. One such promising reaction is the atom-economical conversion of CO_2 with epoxides into cyclic carbonates, which can then serve as precursors to polymers, pharmaceuticals, and other high-value materials. This process can be catalyzed by transition-metal catalysts or organocatalysts. Organocatalysts, as opposed to traditional metal-based catalysts, present a greener, more sustainable option due to their lower cost, reduced toxicity, and wider functional diversity. However, current organocatalysts often suffer from lower efficiency, limiting their industrial application. This project seeks to overcome this barrier by employing a data-driven, computational approach to optimize organocatalysts that can efficiently activate CO_2, transforming it into a valuable feedstock for various chemical processes.

This project will use *state-of-the-art* computational methods to identify and understand trends in reactivity of organocatalysts for the reaction of epoxides with CO_2, with the aim of optimizing their activity, to achieve highly efficient novel catalysts. The project will combine advanced computational chemistry with data-driven methodologies to achieve the desired catalyst optimization.

Methodology

This project will leverage *state-of-the-art* electronic structure methods, data analysis, and machine learning techniques to unlock new structure-activity relationships, guiding the rational optimization of catalysts to achieve unprecedented efficiency.

Training

The PhD student involved in this project will receive comprehensive training comprising both computational methods for electronic structure computations, machine learning, and data analysis.

The student will have the chance to acquire expertise in usage of high-performance computing resources, writing Python code and application of machine learning to molecular structures. As the use of machine learning and AI has been growing rapidly in recent years, and its influence on chemistry is becoming more and more pronounced, the acquired skills from this project can place the student at the forefront of modern chemical research, positioning them as future leaders in both academia and industry.
The research plan of the PhD will provide the student with opportunities for participating in research conferences and workshops. These can include CCP5 summer school on computing, as well as AI tailored training by the AiChemy Hub (https://aichemy.ac.uk).

References

1. E. Solel, N. Tarannam and S. Kozuch, *Chem. Commun.*, 2019, **55**, 5306–5322.
2. M. D. Wodrich, B. Sawatlon, E. Solel, S. Kozuch and C. Corminboeuf, *ACS Catal.*, 2019, **9**, 5719–5725.
3. N. T. Runcie and A. S. J. S. Mey, *J. Chem. Inf. Model.*, 2023, **63**, 5996–6005.

For further information on the project – Project | E5 Doctoral Training Partnership | E5 Doctoral Training Partnership

Application Process

More information on the application process is available on the E5 DTP website – How to Apply | E5 Doctoral Training Partnership | E5 Doctoral Training Partnership

Closing date: 14th December 2025 (midnight, GMT)

In the first instance, the initial application of cover letter and CV should be directed to: Ephrath.solel@ed.ac.uk

IMPORTANT

Before Submitting your cover letter and CV, please complete the online **School of Chemistry Equality, Diversity & Inclusion Form for 26/27 Entry**

The form will automatically generate a unique 'Receipt Number' that you must include in your cover letter.

Equality and Diversity

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality. The University has a range of initiatives to support a family friendly working environment. See our University Initiatives website for further information. University Initiatives website: https://equality-diversity.ed.ac.uk/inclusion/family-and-carer