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 E5 DTP at the University of Edinburgh and covers tuition fees and an annual stipend at the UKRI rate, this is currently £19,237 per annum for 2024-2025.

For entry requirements and eligibility criteria, please see:

Entry and Eligibility Criteria | E5 DTP

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 catalysed 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 in 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 methods to unlock new structure-activity relationships, guiding the rational optimization of catalysts to achieve unprecedented efficiency and effectiveness.

For further information on the project, please see:

Project | E5 DTP

Application Process

For more information on the application process, please see the E5 DTP website:

Application Process | E5 DTP

The application deadline is Monday 6 January 2025 at 12:00 noon, GMT

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.

For further information, please see our University Initiatives website:

https://equality-diversity.ed.ac.uk/inclusion/family-and-carer