Centre for **Sustainable & Circular** Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Nanoscale Reaction Mapping for the Rational Design of Biomass Conversion Catalysts
Supervisors at Bath:	Dr Simon Freakley, Prof Frank Marken
Supervisors at Monash:	Dr Cameron Bentley
Home Institution:	Bath
Indicative period at Host Institution:	12 months

Project Summary

The catalytic conversion of sustainable biomass into value added chemicals via selective reduction and oxidation (redox) reactions is a key enabling technology in the transition to a sustainable chemical sector. To develop more efficient catalytic processes, a greater fundamental understanding of structure–activity relationships is required; especially under aqueous reaction conditions which are desirable for biomass conversions to reduce separation costs. This project will develop tools to design new redox catalysts using electrochemical half reactions as a screening tool with direct imaging of catalytic activity at the nanoscale for the first time, to identify the most active structures present on a heterogenous (electro)catalyst surface.

Performing these redox reactions in aqueous media opens new reaction pathways involving the movement of charged species at metal-liquid interfaces. For instance, in the oxidation of glycerol, the role of molecular O2 is to accept electrons from the catalytic nanoparticle (akin to electrochemical oxygen reduction) rather than be incorporated directly into the products.1 Similarly, aqueous HMF hydrogenation has been shown to involve water-mediated protonation (driven by H2 oxidation) rather than direct interaction with surface bound H species.2 These studies suggest that biomass conversion can be broken down into coupled elementary steps such as H2 oxidation - carbonyl reduction, O2 reduction - C-H oxidation and dehydrogenation – H + reduction and this could provide new approaches to catalyst design and understanding in these important processes.

This project will combine expertise in heterogeneous catalysis (Freakley), electrochemistry (Marken), and state-of-the-art reaction imaging down to the sub-single nanoparticle level (Bentley), to develop new tools to design and understand heterogeneous catalysts based on metal nanoparticles for biomass conversion. We will test the hypothesis that biomass conversions can be modelled as coupled redox processes—through the testing of isolated half reactions electrochemically to predict the optimum catalyst structures as a synthetic target. The project will utilize nanoscale high-resolution electrochemical microscopy to directly image the sites that promote effective catalysis of these essential half reactions. Ultimately, relating electrochemical activity on this scale to the underlying structure will guide the design/synthesis of the “next-generation” of materials with higher activity, improved stability, and longer life – which are all crucial metrics for sustainable catalysis.

1 Zope et al., Science, 2010 (330) 74-78 2 Zhao et al., Nature Catalysis, 2019, (2), 431-436

Features of the programme

- PhD researchers will be registered at both institutions and will be awarded a joint PhD degree.
- PhD researchers will be jointly supervised by academics from both Monash and Bath Universities.
- All PhD researchers in the joint programme will also undertake a bespoke advanced training plan covering a range of topics focusing on sustainability.
- Applicants can apply to either Monash University or the University of Bath as their nominated home institution.
- PhD researchers will undertake a period of no less than 12 months at the partner institution.
- Up to four scholarships/studentships will be offered. Additional and suitably qualified applicants who can access a scholarship/studentship from other sources will be also considered. Evidence of funding must be provided.
- The scholarships/studentships include:
  - a *full tuition fee sponsorship* provided by Monash or Bath for the course duration (up to a maximum 42 months). Note, however, that studentships for Bath-based projects will provide cover for UK/EU tuition fees ONLY.
  - *a living allowance (stipend)* provided by Monash or Bath Universities.

Note: Overseas Student Health Cover (OSHC) must be paid by the student, unless covered by the university.

How to apply

You MUST express interest for three projects in order of preference. Please submit your application at the Home institution of your preferred project ('Home' institution details can be found in the project summary). However, please note that you are applying for a joint PhD programme and applications will be processed as such.

The deadline to submit applications is 30th January 2022

Monash University

Expressions of interest (EoI) can be lodged through https://www.monash.edu/science/bath-monash-program. The EoI should provide the following information:

CV including details of citizenship, your Official Academic Transcripts, key to grades/grading scale of your transcripts, evidence of English language proficiency (IELTS or TOEFL, for full requirements see: https://www.monash.edu/graduate-research/faqs-and-resources/content/chapter-two/2-2), and two referees and contact details (optional). You must provide a link to these documents in Section 8 using Google Drive (Instructions in Section 8).

University of Bath

Please submit your application through the following link: https://www.csct.ac.uk/bath-monash-global-phd-programme/

Please make sure to mention in the "finance" section of your application that you are applying for funding through the joint Bath/Monash PhD programme for your specified projects.

In the "research interests" section of your application, please name the three projects you are interested in and rank them in order of preference. Please also include the names of the Bath lead supervisors.