Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	eGas: Direct Electrocatalytic Generation of CO and H_2 from Renewables
Supervisors at Bath:	Dr Ulrich Hintermair, Prof. Frank Marken
Supervisors at Monash:	Dr Cameron Bentley
Industrial partner:	Dr Nicholas van Dijk (Oort Energy)
Home Institution:	Bath
Indicative period at Host Institution (Monash):	12 months

Project Summary (to include a brief description of the relevance to sustainable & circular technologies)

Mixtures of CO and H_2 (syngas) are a core feedstock of the chemical industry to synthesise a variety of important bulk chemicals and commodities such as methanol, acetic acid, fuels and lubricants. Currently produced from methane steam reforming or coal gasification (on a global scale of ~600m tons), syngas is derived from fossil resources and responsible for ~5% of global CO_2 emissions. Access to clean syngas based on renewables would enable the production of sustainable net zero carbon fuels and chemicals akin to Asinger's vision of a future methanol economy. Efforts to produce green H_2 from water electrolysis powered by renewable energy on large scale are underway, but access to sustainable carbon sources such as green CO remains challenging. While in principle, green H_2 could be used to reduce CO_2 from the air (either electrochemically or via traditional water-gas-shift chemistry), the entropic penalty associated with direct air capture technologies at ~400 ppm concentration means that the overall process efficiencies are very low. Syngas production from biomass or other waste streams *via* anaerobic digestion is a promising alternative which does not rely on capturing carbon from the air. However, due to the low production rates and lack of selectivity control, microorganism-based digestion processes are not well suited to produce clean syngas on a large scale.

Given that O_2 evolution is the kinetically limiting factor of electrocatalytic water splitting, and that CO_2 capture and reduction is inefficient, we propose to design new electrocatalytic materials that selectively electrolyse renewable carbon feedstocks such as biomass and waste directly to CO and H_2 (eGas). Such a cell would produce valuable products in both half-reactions (avoiding the anodic co-generation of undesired O_2 and CO_2) directly from low-value starting materials using renewable electricity as the only energy input. Key to this will be designing new electrode materials that selectively oxidise organic molecules to CO under conditions where cathodic proton reduction may occur. This area is not well understood and has rarely been investigated in the literature but there are some leads on suitable materials such as Ni foam electrodes.

In this project we will design, synthesise and test electrocatalyst materials for the selective, partial oxidation of oxygenated model compounds such as ethylene glycol and carbohydrates as a starting point. As a key prerequisite for controlling the processes occurring in such cells is a comprehensive understanding of the solution and headspace composition under working conditions, the project will make use of one of the most advanced setups for real-time reaction monitoring in the DReaM Facility at Bath. FlowNMR techniques paired

with real-time headspace mass spectrometry and other methods will give insight into reaction selectivity as a function of potential, time, pH, feed etc. to quickly identify promising materials and operating conditions. ^{2}H, ^{13}C and ^{18}O isotopic labelling techniques and kinetic analyses will further help to elucidate the mechanism and rationalise reaction pathways to each product observed. Further understanding of the working principles of the catalyst itself will come from tempo-spatial surface mapping with *in situ* electrochemical microscopy during your time spent at Monash. Our industrial partner Oort Energy (an innovative electrolyser company who are about to open a new site between Bath and Bristol) is very keen to become involved in this project and offers advice on applied aspects of cell configuration, membrane materials and device operation including industrially relevant metrics and targets.

Due to the novelty of this project and combination of cutting-edge techniques there is ample scope for high-impact publications and excellent training opportunities for the student despite it being ambitious, early-stage research.

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 2023

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.