

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Sustainable Water Splitting Using Electrocatalysts with Isolated Atomic Sites
Supervisors at Bath:	Prof Frank Marken / Dr Ulrich Hintermair
Supervisors at Monash:	Dr Jie Zhang (lead) / Dr Cameron Bentley
Home Institution:	Monash
Indicative period at Host Institution:	12 months

Project Summary

*Water splitting by electrolysis* is recognised to be one of the most promising approaches to convert and store renewable electricity in the form of hydrogen as a way to reduce our overreliance on non-renewable fossil fuels. To overcome high intrinsic energy barriers associated with this seemingly simple reaction, commercially viable water electrolysis requires the use of highly active and stable nanostructured electrocatalysts on both electrodes, such as porous films or nanoparticles with high surface-area-to-volume-ratios. Ideally however, all active atoms of the catalyst should be exposed to the reactants in solution and connected to the circuit to contribute to the catalysis as for example in natural enzymes. This is particularly important for rare/expensive precious metals, such as Pt, Pd, Ir, Ru, used for water electrolysis in acidic media. The ongoing search for low-cost, earth-abundant alternatives has spawned novel classes of material with well-defined, isolated active sites, for example single atom catalysts (SACs) and immobilised molecular catalysts (IMCs). While SACs and IMCs are optimal in terms of atomic utilisation, understanding catalytic mechanisms and the pathway(s) of catalyst deactivation on this scale is an ongoing challenge due to limitations in conventional instrumental approaches.

This PhD will introduce new paradigms for the fabrication and *operando* characterisation of SAC and IMC electrocatalyst materials by leveraging capabilities from Monash (electrochemistry, electrochemical imaging, electromaterials) and Bath (electrochemistry, spectroscopy, inorganic synthesis) and will:

- (i) Devise new methods to prepare highly-active, low-cost and ideally earth-abundant SACs and IMCs for use in water electrolysis;
- (ii) Use Monash and Bath-specialised, advanced (spectro)electrochemical characterisation tools with high spatiotemporal resolution to probe the active site(s) *in situ* during catalytic turnover, developing an in-depth understanding of catalytic activity/mechanisms;
- (iii) Perform complementary, advanced X-ray spectroscopy with the synchrotron light source to observe the potential- and/or time- dependent active site structure/composition in *operando*;
- (iv) Use the information from (i-iii) to engineer “next-generation” SACs/IMCs with enhanced function (*e.g.*, high activity, stability *etc.*), which will be tested under commercially-relevant conditions in a gas-diffusion electrode (GDE) setup.

The work aligns with sustainable and circular technologies since it aims to produce novel, low-cost, earth-abundant catalysts with isolated active sites that effectively minimizes/eliminates the need for rare precious metals in water electrolysis, addressing key research challenges spanning chemistry, material science and engineering. The work will contribute to Australia’s National Hydrogen Strategy, which “sets a vision for a clean, innovative, safe and competitive hydrogen industry that benefits all Australians. It aims to position our

industry as a major player by 2030" (<https://www.industry.gov.au/data-and-publications/australias-national-hydrogen-strategy>). Monash will provide expertise in SAC synthesis and advanced electrochemical characterisation at the macroscale (Zhang) and nanoscale (Bentley), while Bath will provide expertise in inorganic synthesis and NMR spectroscopy (Hintermair) and electrochemical and Raman spectroscopic characterisation (Marken). Once commercially viable water electrolysis technologies are developed, the feasibility for industrial applications will be explored through collaboration with industrial partners, such as Woodside Energy through the Monash-Woodside partnership, taking advantage of their well-established and readily available commercialization mechanisms.

### 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 11th April 2021**

#### **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.