

Bath Monash Global PhD Programme in Sustainable Chemical Technologies

Project Title:	Molecular surface species and mechanism in energy conversion
Supervisors at Bath:	Dr Ulrich Hintermair (lead) and Prof. Frank Marken
Supervisors at Monash:	Dr Jie Zhang
Home Institution:	University of Bath
Indicative period at Host Institution:	From October 2020 to September 2021

Project Summary

Understanding electron transfer processes at solid-liquid interfaces (i.e. electrode surfaces) is key to efficient renewable energy conversion, such as wind- or solar-powered electrolysis of water to generate clean energy vectors such as hydrogen. The molecular approach is an alternative to fabricating monolithic materials and a way of gaining better control over the kinetics of electrocatalytic charge transfer at the interface (analogous to biological processes). Here, the use of tailored-made molecular adsorbates is envisaged on the surfaces of cheap and abundant electrode materials such as graphite. Using molecular electrocatalysts that can be synthesized and characterized in solution before being mono-layer deposited onto suitable electrodes offers many advantages over traditional alternative approaches. In this project we will combine key expertise in the quantitative study of electrocatalysis and electroanalysis (Zhang), molecular catalysis for energy conversion (Hintermair), and (nano)electrochemistry and sensing (Marken) to develop new molecular materials for selective and efficient energy conversion schemes including those needed in water splitting, CO<sub>2</sub> and heterocycle reduction, and in N<sub>2</sub> activation.

Example publications:

[“Graphene-Supported  \$\[\{Ru\_4O\_4\(OH\)\_2\(H\_2O\)\_4\}g-SiW\_{10}O\_{36}\]^{10-}\$  for Highly Efficient Electrocatalytic Water Oxidation”](#)

S.-X. Guo, Y. Liu, C.-Y. Lee, A.M. Bond, J. Zhang,\* Y.V. Geletii, C.L. Hill\*

Energy Environ. Sci. **2013**, 6, 2654 - 2663.

[“A Molecular Catalyst for Water Oxidation that Binds to Metal Oxide Surfaces”](#)

S. W. Sheehan,\* J. M. Thomsen, U. Hintermair,\* R. H. Crabtree, G. W. Brudvig,\* C. A. Schmuttenmaer

Nature Communications **2015**, 6, 6469.

[“Electrochemical and Kinetic Insights into Molecular Water Oxidation Catalysts Derived from Cp\\*Ir\(pyalk\) Complexes”](#)

E. V. Sackville, F. Marken, U. Hintermair\*

ChemCatChem **2018**, 10 (19), 4280–4291.

[“The thermoelectrochemistry of the aqueous iron\(ii\)/iron\(iii\) redox couple: Significance of the anion and pH in thermogalvanic thermal-to-electrical energy conversion”](#)

M. A. Buckingham, F. Marken,\* L. Aldous\*

Sustainable Energy and Fuels **2018**, 12, 2717-2726.

## 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 Bath (home or EU students only) or Monash for the course duration (up to a maximum 42 months)
  - *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.

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## How to apply

Please express interest for up to three projects in order of preference. Please submit your application at the Home institution of your preferred project. 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 Sunday 12 May.**

### ***Monash University***

Expressions of interest (Eoi) can be lodged through <https://forms.gle/XkC1TKpqVQh4B4N1A>. The Eoi should provide the following information:

CV including details of citizenship, full transcripts of academic records, evidence of English language level (IELTS or TOEFL), nominate your host institution (ie Bath or Monash), two referees and contact details, indication of which projects are of interest.

### ***University of Bath***

Please submit an application through the following link:

[https://samis.bath.ac.uk/urd/sits.urd/run/siw\\_ipp\\_lgn.login?process=siw\\_ipp\\_app&code1=RDUCH-MO01&code2=0001](https://samis.bath.ac.uk/urd/sits.urd/run/siw_ipp_lgn.login?process=siw_ipp_app&code1=RDUCH-MO01&code2=0001)

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 up to three projects you are interested in and rank them in order of preference. Please also include the names of the Bath lead supervisors.