Centre for **Sustainable** Chemical Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable Chemical Technologies

Project Title:	Molecular surface species and mechanism in energy conversion
Supervisors at Bath: Supervisors at Monash:	Dr Ulrich Hintermair (lead) and Prof. Frank Marken 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_2 and heterocycle reduction, and in N_2 activation.

Example publications:

"Graphene-Supported [{$Ru_4O_4(OH)_2(H_2O)_4$}g-$SiW_{10}O_{36})_2$]$^{10-}$ 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.