Centre for **Sustainable & Circular** Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Redox mediated nitrogen reduction to ammonia: a mechanism-guided approach to developing new catalysts for a sustainable future
Supervisors at Monash (Home institution)	Dr Alexandr N. Simonov Prof Douglas R. MacFarlane
Supervisors at Bath (Host institution)	Dr Ulrich Hintermair
Indicative period at Bath	2nd year

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

Ammonia is among the most significant industrial chemicals, that feeds the humanity through the fertiliser industry underpinned by this single simple molecule. NH_3 is also considered as a sustainable hydrogen carrier and fuel of the future, which combustion would release only pure N_2 and water. Current methods for the ammonia synthesis are strongly polluting, which motivates the development of new sustainable technologies, like renewable-powered electrosynthesis. The PhD project will aim to advance the current most promising redox-mediated electrochemical technology for the ammonia electrosynthesis from dinitrogen and water thorough investigation of the mechanism and kinetics of the reaction mediated by molecular and heterogeneous electrocatalytic systems. This includes a combination of cutting-edge electrochemical characterisation techniques, *operando* spectroscopy of working electrolyte solutions, and *in situ* catalyst characterisation by spectroscopic techniques. The supervisory team offer expertise in all relevant areas, spanning the range from molecular synthesis to applied electrocatalysis, and the PhD candidate will develop world-class skills by applying these to a high impact project of intense current interest.

Research task include (but are not limited to):

(1) Synthesis of organometallic complexes as molecular redox mediators for the N_2 reduction;

(2) Characterisation of redox mediators using advanced electrochemical and spectroscopic techniques;

(3) Chemical and electrochemical N_2 reduction experiments;

(4) *Operando* investigation of the N_2 reduction kinetics using advanced high-field FlowNMR spectroscopy at Bath and *in situ* XAS at the Australian Synchrotron and BESSY II synchrotron.

(5) Modelling and automated fitting of the (electro)chemical kinetics data.

The project is flexible and specific research tasks can be adjusted to match the strengths and interests of the PhD candidate.