Centre for Sustainable Chemical Technologies

UNIVERSITY OF BATH

Centre for Sustainable Chemical Technologies; University of Bath

Project Title:	Reactions in Deep Eutectic Solvents: Time-resolved studies of structure control via solvent bonding
Lead Supervisor:	Professor Karen Edler (Department of Chemistry)
Co-supervisor:	Dr Daniel Bowron (ISIS)
Industrial Partner:	ISIS Neutron and Muon Science (Science and Technology Facilities Council)

Project Summary

Deep eutectic solvents (DES) have recently emerged as exciting alternatives to replace toxic organic solvents with cheap, environmentally benign, bio-inspired liquids in a range of chemical processes. DES provide substantial improvements in chemical reactions, allowing, for example, formation of inorganic oxide nanomaterials at much lower temperatures, and milder synthesis conditions than standard reactions in water. In addition, DES allow air- and water-sensitive chemical reactions to proceed at room temperature under normal atmospheric conditions – a huge improvement in safety and cost. Inorganic nanomaterials are key to technologies such as hydrogen fuel production from water and pollution remediation but greener routes to such materials are needed to ensure they themselves can be produced in a sustainable manner. Low temperature synthesis in biodegradable, renewable solvents such as DES will be key to designing structured materials for such applications. Yet, so far surprisingly little is understood about *how* DES structures and interactions with solutes facilitate such reactions and whether solvent properties such as chirality or nanophase separation can be used to affect their properties. This project aims to understand how solvent structures and interactions with solutes influence reactivity in DES and so can control growth of inorganic nanoparticles for (photo)catalysis.

This is a multidisciplinary project combining nanoparticle synthesis with experimental techniques for solvent and nanostructure characterisation including time-resolved wide-angle neutron scattering experiments in combination with modelling, and other *in situ* experiments such as small angle scattering and NMR to study the evolution of the solvent and reactants/products on molecular and nanoscales with time. Molecular solvent structures and interactions with solutes will be probed using NMR, wide-angle neutron scattering, and EXAFS for inorganic species, while nanoparticle growth and nanoscale structuring will be studied using small angle X-ray and neutron scattering. Nanoparticles and porous materials will be studied using electron microscopy, gas sorption and XRD, as well as evaluation of their (photo)catalytic properties (eg solar water splitting to create hydrogen). DES will also be characterised via surface tension, viscosity, light scattering and thermal properties (DSC). Since this is a collaborative project between the University of Bath and the ISIS Neutron Scattering Facility the student will spend part of their PhD working at the Rutherford Appleton Lab at the ISIS Spallation Source. The student will also be expected to travel to neutron and synchrotron X-ray facilities in the UK, France and possibly the USA or Australia as part of their PhD work.

Sustainability issues addressed

By advancing knowledge on how solvent structures and interactions with solutes influence reactivity in DES, this project has the potential to make chemical processes more sustainable – cheaper and safer for the environment - and accelerate the adoption of DES as alternatives to replace toxic organic solvents.