

Bath Monash Global PhD Programme in Sustainable Chemical Technologies

Project Title:	Can ionic liquids revolutionise sustainable polymers?
Supervisor at Bath:	Dr Antoine Buchard (lead)
Supervisor at Monash:	Professor Katya Pas
Home Institution:	University of Bath
Indicative period at Host Institution:	From October 2020 to September 2021 and from April 2022 to September 2022

Project Summary

Context: Polymers and the problems associated with their use and disposal have recently fallen into the public eye, driving even further research into sustainable plastic materials. In particular, polymers from renewable resources alleviate polymer dependence on fossil fuel feedstocks and can impart enhanced degradability and chemical recyclability to the resulting materials.

Challenges addressed: Ring-opening polymerisation (ROP) has been one method of choice to produce sustainable polymers, with the development of hundredths of catalytic systems for lactide and other renewable monomers. However, there has been several limitations to the uptake of novel ROP methods and new monomers by the polymer industry and material scientists: the need for stringent air and moisture free conditions, the limited solubility of highly oxygenated polymers in common solvents (partly driving the need to perform polymerisation at high temperature in melt monomer/polymer mixture), and the detrimental contamination of the plastic recycling chain by new polymers.

Hypotheses: Our hypothesis is that using ionic liquids (ILs) can break those constraints and generalise the use of ROP methods and the uptake of novel renewable polymers by industry and material scientists. ILs are indeed known to solubilise highly oxygenated (macro) molecules and would therefore allow to use established low temperature ROP techniques and achieve high molecular weight polymers. We also propose that the known presence of polar and non-polar domains in ILs would remove the need for air/moisture-free conditions, by creating confined nano-reactors in the reaction mixture, isolating detrimental impurities like water. Finally, based on literature precedent and on their similarity with acid:base complexes often used in ROP, ILs themselves could act as polymerisation catalysts, easily tuneable to control kinetic rates and the polymerisation outcomes, including polymer microstructure and sequence.

Project: These hypotheses will be tested using a joint experimental (Bath) and computational (Monash) approach. In particular, based on the existing model developed by the Pas group for radical polymerisation in ILs, we will develop and validate a general predictive framework for ROP processes of renewable polymers in ILs, including sugar-based structures developed in the Buchard group. We will then gain the ability to predict and carry out selective and controlled polymerisation of renewable monomers with and in ILs, under non-stringent conditions.

Outcomes and Impact: This project will open up new possibilities for sustainable polymer manufacturing: lower energy requirements and less constricting conditions, efficient recovery/purification of polymers post-synthesis, direct additive manufacturing of ionic liquid/polymer gels, e.g. for electronic applications. Moreover, as it will rely on similar chemistry, we will be able to apply our findings to the selective chemical

recycling and upcycling of mixed plastic waste (e.g. PET, PEF, PC, PLA mixtures), decontaminating recycling streams and working towards a circular economy of plastics.

Synergies with other CSCT and Monash research groups: Prof Janet Scott (Bath; ILs for biopolymer processing), Prof Matt Davidson (Bath; PEF and PLA catalysis) Prof Douglas MacFarlane (Monash; energy applications of ionic gels), Prof Tanya Junkers (Monash; flow processes for polymer synthesis).