Centre for **Sustainable & Circular** Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Precise, Rapid and Scalable Sustainable Polymer Synthesis by Automated Catalytic Flow Reactors
Supervisors at Bath:	Dr Antoine Buchard (lead)
Supervisors at Monash:	Prof Tanja Junkers
Home Institution:	University of Bath
Indicative period at Host Institution:	2.5 years at Bath; 1 year at Monash with exact dates to be confirmed

Project Summary

Polymers and the problems associated with their misguided use and disposal have recently fallen into the public eye, and are driving further research into sustainable plastic materials. One vision for sustainable polymers is that of a class of materials, derived from renewable feedstocks, which exhibit closed-loop life cycles, including enhanced degradability and chemical recyclability. The synthesis of some of these renewable polymers (*e.g.* poly(lactic acid), arguably one of the success story in this field) occurs industrially via the ring-opening polymerisation (ROP) using a homogeneous tin(II) based catalyst, which has been for a long time under scrutiny because of residual toxicity concerns. Using heterogeneous catalysts for ROP, in particular under industrially relevant solvent free conditions, is a promising strategy to limit residual metal content, but also to propose new ways of manufacturing these polymers.

Recently, at Bath, the Buchard group (www.buchargroup.org) has developed single site metal complexes immobilised onto an inert poly(styrene) support, which are very active and fast ROP catalysts, display excellent polymerisation control, can be reused and leave little metal residue behind.[1] Furthermore, these catalysts are ideally suited to be translated from batch to flow processes and to disrupt the established production of polymers made by ROP. In Monash, the Junkers group (www.polymatter.net) specialises in the precise engineering of polymers using flow processes and on-line analysis of polymerisation reactions.[2] Recently, they have developed a continuous flow system for automated high-throughput screening and autonomous optimisation of radical polymerisations. This platform comprises a flow reactor coupled to size exclusion chromatography (SEC), and is controlled by a machine-learning algorithm that continuously vary reaction parameters until target molecular weights are achieved.[3-4]

In this project, we aim to build on some preliminary collaborative interactions (including the short secondment of a PhD student from the Buchard group in Monash) and investigate if autonomous flow polymerisation processes can be applied to ROP reactions, including using some novel heterogeneous catalysts and some novel monomers from sugars.[5-6] This will not only propose a new way to produce these sustainable polymers, but also allow to rapidly and precisely create a wide range of polymers for analysis, so that improved materials can be developed using an efficient feedback loop. In addition, by adjusting reactions conditions further, the autonomous set-up and the catalysts developed will also be amenable to depolymerisation studies, so as to assess the potential of promising renewable polymers for chemical recycling.

The student will be based in Bath, and they will initially work with Dr Buchard to develop and apply abundant metal and metal- free supported catalysts for the ring-opening polymerisation of cyclic carbonates and cyclic

esters, first in batch and then in flow set-ups. These catalysts will be studied using in-situ IR spectroscopy as well as on-line NMR analysis, using Bath DReaM facilities (www.bath.ac.uk/research-facilities/dynamic-reaction-monitoring-facility/). During their year in Monash, supervised by Prof Junkers, they will couple these catalytic systems with an on-line Size Exclusion Chromatography (SEC) and use a machine-learning algorithm to self-optimise reactions conditions towards programmed molecular weights and molecular weight distribution shapes. An on-line set-up will then be implemented back in Bath, and used for the rapid, scalable and precise synthesis of various sustainable polymers, so as to get a deeper understanding of their structure/property relationship and inform future monomer design. Depolymerisation studies will also be initiated.

References:

1) I. C. Howard, C. Hammond and A. Buchard, *Polym. Chem*. 2019, *10*, 5894-5904.
2) T. Junkers, *J. Flow. Chem* 2018, *7*, 106-110
3) M. Rubens, J.H. Vrijsen, J. Laun and T. Junkers, *Angew. Chem. Int. Ed.* 2019, *58*, 3183-3187
4) M. Rubens and T. Junkers, *Polym. Chem.* 2019, *10*, 6315-6323.
5) T. M. McGuire, C. Pérale, R. Castaing, G. I. Kociok-Köhn and A. Buchard, *J. Am. Chem. Soc.* 2019, *141*, 13301-13305.
6) G. L. Gregory, L. M. Jenisch, B. Charles, G. I. Kociok-Köhn, A. Buchard, *Macromolecules* 2016, *49*, 7165-7169.

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 Monash or Bath for the course duration (up to a maximum 42 months). Note, however, that studentships for Bath-based projects will provide cover for UK/EU tuition fees ONLY.
  - *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.

How to apply

You MUST express interest for three projects in order of preference. Please submit your application at the Home institution of your preferred project ('Home' institution details can be found in the project summary). 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 23rd February 2020

Monash University

Expressions of interest (EoI) can be lodged through https://www.monash.edu/science/bath-monash-program. The EoI should provide the following information:

CV including details of citizenship, your Official Academic Transcripts, key to grades/grading scale of your transcripts, evidence of English language proficiency (IELTS or TOEFL, for full requirements see: https://www.monash.edu/graduate-research/faqs-and-resources/content/chapter-two/2-2), and two referees and contact details (optional). You must provide a link to these documents in Section 8 using Google Drive (Instructions in Section 8).

University of Bath

Please submit your application through the following link: https://www.csct.ac.uk/bath-monash-global-phd-programme/

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