Centre for **Sustainable & Circular** Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Bio-derived materials with enhanced properties: controlling the composition of bioderived polymers through automation and machine learning
Supervisors at Bath:	Dr Antoine Buchard, Dr Hannah Leese
Supervisors at Monash:	Prof Tanja Junkers
Home Institution:	Bath
Indicative period at Host Institution:	18 months

Project Summary

The reliance of plastic materials on fossil resources and concerns about their end of life necessitate a transition to a circular economy of plastics. One vision for sustainable plastics is that of a class of materials, derived from renewable feedstocks, which exhibit closed-loop life cycles (mechanical and chemical recyclability and/or biodegradability). However, a major technological barrier limiting the widespread adoption of polymers from renewable feedstocks is the need to achieve a delicate balance between thermomechanical performance and degradability.

One strategy used to tune the properties of polymeric materials is the copolymerisation between two or more monomers, combined with the control of the composition and sequence of the resulting copolymers. This usually necessitates the determination of monomers relative reactivity ratios, which is a lengthy and labour-intensive process. In addition, the differences in intrinsic reactivities of monomers means that it can be extremely challenging to achieve specific sequences, in particular statistical copolymers. Unfortunately, these challenges considerably limit our ability to discover new materials that could address technological needs (e.g., materials with high gas barrier properties but with embedded or triggerable degradability).

In particular, at Bath, the Buchard group (www.buchargroup.org) has been developing a platform of monomers and polymers derived from sugars.[1-3] These renewable and degradable materials have shown promise for a variety of applications, including packaging, battery solid electrolytes and health materials (in collaboration with the Leese group (www.materialsforhealthlab.org). Considering the diversity of sugar feedstocks, and the possibilities offered by copolymerisation, the structure/property space to explore is immense and necessitates a rational and optimised approach.

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. Recently, they have for example developed a continuous flow system for automated high-throughput screening and autonomous optimisation of radical polymerisations, which is controlled by a machine-learning algorithm that continuously vary reaction parameters until target molecular weights are achieved.[4-5]

In this collaborative and multidisciplinary project, we will develop an experimental set-up which is able to vary copolymerisation reaction parameters (rate of addition, concentrations, temperature etc.) and automatically explore new bio-derived copolymer compositions and sequences, and relate those to the polymer physical properties, which will ultimately inform the design of materials with enhanced characteristics.

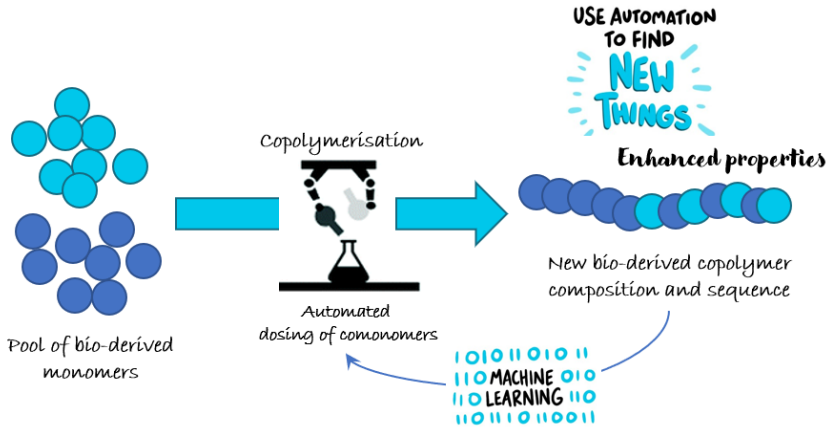

Figure 1. Project overview

Specifically, our objectives will be to:

1) Develop an automated experimental set-up comprising a feedback loop between the analysis of copolymer composition/sequence (e.g., by IR or NMR spectroscopy) and the automated dosing of comonomers (e.g., using syringe pumps), via a combination of online monitoring and machine-learning-based optimisation.
2) Demonstrate the efficacy of such set-ups to efficiently produce bio-derived copolymers (e.g., via ring-opening polymerization) with well-defined and controlled sequence and composition, including hitherto inaccessible ones.
3) Produce charts showing combinations of established and emerging renewable monomers versus their physical properties (thermomechanical performance and degradability).
4) Identify performance gaps and, through a combination of novel synthesis and understanding of structure-property relationships, design and test materials to fill those gaps.

The project will for example study the controlled incorporation of novel bio-derived cyclic monomers (e.g., from sugars) into oxygenated polymers (like PLGA or PLA; see example in figure below), towards more degradable materials that can still perform their intended function (e.g., mechanical). Another target will be to control the amount and location of functionalised comonomers incorporated into the polymer backbone towards the precise synthesis of molecular imprinted polymers for health and catalysis applications.

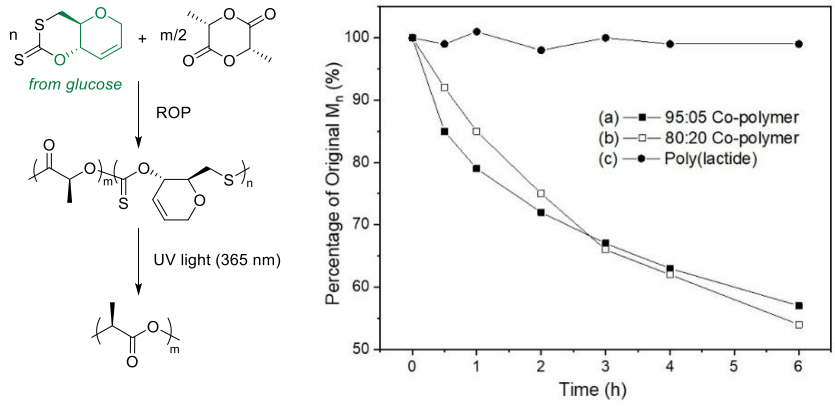

Figure 2. Degradation of copolymers of PLLA (95 or 80% LA) once exposed to UV irradiation (λ = 365 nm).

The student will be based in Bath, and they will initially work to synthesise a pool of renewable monomers and copolymers and develop the appropriate analytical methods to identify their composition and sequence, first in batch and then in flow set-ups. Techniques will include *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 time in Monash, supervised by Prof Junkers, they will combine online composition analysis with a machine-learning algorithm to automate the synthesis of copolymers and self-optimise reaction conditions towards specific composition and sequence. Such set-up will then be implemented back in Bath, and used for the rapid, scalable and precise synthesis of bio-derived polymers with controlled composition and sequence. The physical properties of the resulting polymers will be analysed and novel structure/property relationships revealed, which will inform the design of copolymers able to address unmet needs and specific applications.

References:

1) M. Piccini, J. Lighfoot, B. Castro Dominguez and A. Buchard, *ACS Appl. Polym. Mater.* 2021*, 3*, 5870-5881.
2) T. M. McGuire, E. F. Clark, A. Buchard, *Macromolecules* 2021, *54*, 5094-5105.
3) G. L. Gregory, L. M. Jenisch, B. Charles, A. Buchard, *Macromolecules* 2016, 49, 7165-7169.
4) M. Rubens, J.H. Vrijsen, J. Laun and T. Junkers, *Angew. Chem. Int. Ed.* 2019, *58*, 3183-3187
5) M. Rubens and T. Junkers, *Polym. Chem.* 2019, *10*, 6315-6323.

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 30th January 2022

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.