

Bath Monash Global PhD Programme in Sustainable & Circular Technologies

Project Title:	Real-time online monitoring of controlled radical polymerisations in continuous flow
Supervisors at Bath:	Maciek Kopec, Ulrich Hintermair
Supervisors at Monash:	Prof Tanja Junkers
Home Institution:	Bath
Indicative period at Host Institution:	24 months

Project Summary

The main challenges of modern polymer chemistry are to develop sustainable replacements of commodity plastics and well-defined, functional materials for specialty applications in nanotechnology, energy conversion/storage and biomedicine. Functional polymers can be synthesized by controlled/'living' radical polymerisation techniques such as atom transfer radical polymerisation (ATRP) and reversible addition fragmentation transfer (RAFT) polymerisation which enable the preparation of well-defined macromolecules with unprecedented levels of structural sophistication.^{1,2} However, sustainable synthesis of precision polymers in a fast and reproducible fashion will require new optimized protocols and reaction design.

In this project we will conduct fundamental studies on the synthesis of various polymer architectures (such as branched, stars or brushes) and compositions (i.e. statistical, block or gradient copolymers) using online reaction monitoring in real time. The integrated multi-technique setup at the Dynamic Reaction Monitoring Facility at the University of Bath will allow to precisely follow polymerisations.³ The combination of advanced high-resolution FlowNMR techniques (1D, 2D, homo-nuclear decoupling, diffusion measurements, etc.) with online mass spectrometry and triple-detection online SEC/GPC promises new insights into the formation of precision polymers in real time.

Photoinduced ATRP (photoATRP) and photoinduced-electron-transfer RAFT (PET-RAFT) techniques will be coupled with continuous flow chemistry to prepare well-defined, complex polymer nanostructures.⁴ Detailed kinetic studies enabled by online reaction monitoring will allow to establish principles for rational design of more robust processes and novel materials.⁵ Specifically, temporal control offered by photo-controlled polymerisations combined with the possibility to follow reactions in real time will significantly broaden our fundamental understanding of the formation of complex polymer architectures.

From the Monash side, the continuous flow process for the reactions will be developed and followed up. Online monitoring is an ideal tool for flow polymerisations as it allows to include machine-learning algorithms to create self-optimizing routines and greatly accelerate the targeted screening of reactions. Such an automated approach will both broaden our fundamental understanding of controlled polymerisations and enable sustainable protocols for the synthesis of well-defined polymers.

References: **1.** K. Matyjaszewski, N. V. Tsarevsky, *J. Am. Chem. Soc.* 2014, *136*, 6513; **2.** G. Moad, E. Rizzardo, S. Thang, *Aust. J. Chem.* 2012, *65*, 985; **3.** J. H. Vrijsen, I. A. Thomlinson, M. E. Levere, C. L. Lyall, M. G. Davidson, U. Hintermair and T. Junkers, *Polym. Chem.* 2020, *11*, 3546; **4.** M. Chen, M. Zhong, J. A. Johnson, *Chem. Rev.* 2016, *116*, 10167; **5.** N; **5.** M. Rubens; J. V. Herck; T. Junkers, *ACS Macro Lett.* 2019, *8*, 1437.

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.