Centre for **Sustainable** Chemical Technologies

MONASH University

UNIVERSITY OF BATH

Bath Monash Global PhD Programme in Sustainable Chemical Technologies

Project Title:	Multi-detector online monitoring of precision polymerizations
Supervisor at Bath: Supervisor at Monash:	Dr Ulrich Hintermair Professor Tanja Junkers (lead)
Home Institution:	Monash University
Indicative period at Host Institution:	12 months with exact dates to be confirmed

Project Summary

Automated chemical synthesis using machine learning algorithms is a rapidly growing field of research. While automation is by definition a chemical engineering task, its development holds high potential also form a synthetic side. With automated, computer controlled protocols at hand, synthesis targets become available that typically would not be approachable in classical synthesis. Especially in conjunction with flow chemistry, unprecedented precision can be reached in (macro) molecular design.

At Monash, we recently demonstrated how online-size exclusion chromatography in combination with machine learning can lead to ultra-precise polymer synthesis (see Rubens *et al. Angew. Chem.* 2019), while concomitantly eliminating largely the human factor from synthesis (resulting in high reproducibility and scalability of the obtained processes). With the extensive online-monitoring facility at Bath University, these endeavors can be brought to a higher level of sophistication.

The combined expertise between both institutions should allow for the development of processes that control almost every variable in a polymerization process. Within the proposed PhD thesis, a fully integrated flow process would be established using living/controlled polymerizations to synthesize polymers with extremely high definition. Variables to assess are monomer conversion, molecular weight, dispersity, endgroup chemistry and copolymer composition. This process will then be used to create materials libraries that can be tested either in situ in the Bath facilities, or offline at either institution. Specific synthesis targets include block copolymers, but also more complex macromolecular architectures.