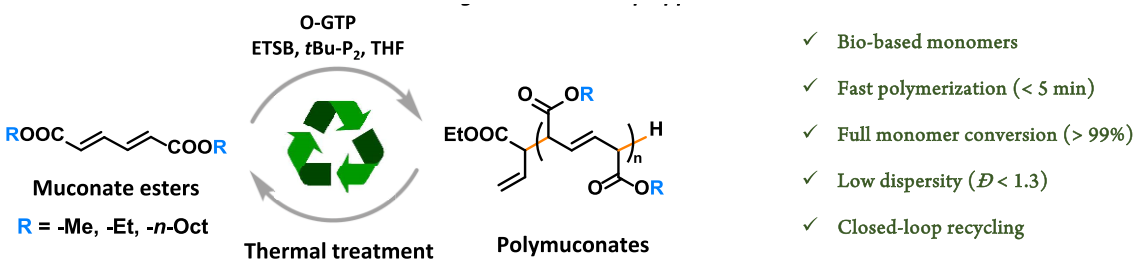
Data-Driven Synthesis of Biobased and Degradable Muconate Polymers in Flow

Scientific Description. Muconate esters are emerging bio-based monomers[1,2] that combine renewable sourcing with a conjugated structure that allows post-polymerization modification and chemical recycling.[3] Group transfer polymerization (GTP) is particularly attractive for their polymerization, providing well-defined polymers under mild, metal-free conditions.[4,5] However, the very high polymerization rates involved make conventional kinetic studies challenging.



This project will exploit the AMETHYST automated flow-chemistry platform[6,7] to investigate the GTP copolymerization kinetics of a series of dialkyl muconates. Continuous-flow experiments will be used to map monomer conversion and copolymer composition as a function of feed composition, allowing determination of monomer reactivity ratios and establishment of structure–reactivity relationships. The resulting kinetic understanding will be used to control copolymer composition and tune the mechanical properties of the resulting materials.

In parallel, Bayesian optimization will be coupled with automated experimentation to achieve targeted molecular and compositional characteristics, building on our work on optimization of ring-opening polymerizations in flow.[7] If time permits, the thermal depolymerization of selected copolymers will also be investigated to assess the relationship between copolymer structure, properties and chemical recyclability.

Techniques. Continuous-flow polymerization using the AMETHYST automated flow chemistry platform; design of experiments (including D-optimal experimental design) for kinetic studies and determination of copolymerization reactivity ratios; Bayesian optimization for data-driven optimization of polymerization conditions; polymer characterization by NMR spectroscopy and size-exclusion chromatography (SEC/GPC); thermal characterization by differential scanning calorimetry (DSC).

Desired Profile. A background in organic or polymer chemistry is desirable. The project involves automated experimentation and data analysis, so an interest in computational methods and a willingness to learn basic coding are important; prior programming experience is not required.

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References.

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