Computational Research in Boston and Beyond Seminar

A Data-Driven Framework for Predicting Frontal Polymerization from Monomer Structure

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12:00 PM - 1:00 PM

Zoom: https://mit.zoom.us/j/91933017072

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Abstract

While thermoset materials offer excellent performance, such as in renewable energy and aerospace applications, they are energy-intensive to make. Only a limited set of monomer chemistries have been identified as amenable to more energy efficient production via frontal polymerization. To learn the governing design principles and optimize for more sustainable high-performance polymer materials, it is critical to link the non-equilibrium process of front polymerization with a given monomer choice. We developed computational pipelines to learn how molecular structure informs the ability of a monomer resin to undergo energy-efficient manufacturing, specifically through frontal ring opening metathesis polymerization (FROMP). In our virtual automated workflow, we combinatorically enumerate candidate monomers and subsequently calculate key reaction parameters from first principles using density functional theory (DFT). We then integrate atomistic chemical insights into a mechanism-based reaction-diffusion model that simulates front propagations. This approach allows us to detail design rules for monomer choice and predict the suitability of a wide range of monomers for FROMP, purely from computation. Overall, our data-driven framework enables rapid processing and screening of new candidates, providing a foundation for *in silico* evaluation and discovery of FROMP amenable materials.