Summer School on Polymeric Networks for Sustainable Development

July 6th – 12th, 2025

Simulating Associative Polymer Networks Far From Equilibrium

T. O'Connor

thomaso@andrew.cmu.edu

This lecture will cover recent developments in the modeling of associative networks during nonlinear flows.
Recent developments in both analytic models and molecular simulations will be discussed, but MD simulations will be emphasized.
The lecture will provide a brief overview of NEMD simulation techniques for modeling nonlinear flow and then demonstrate application of NEMD simulations to associative network systems of varying architecture, association strength, and association coordination.
We will use simulations to explore how associative chain conformations respond to flow and how these dynamics differ from unassociative melts.
One major idea I hope to convey to the students is that the mean-field descriptions we use to describe associative network dynamics in equilibrium can easily break down during nonlinear flow.