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Hosted by the Department of Chemical Engineering

Distinguished Seminar Speaker

Molecular Dynamics Investigations of Thermosetting Polymers

Prof. Cameron Abrams

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Drexel University | Philadelphia, PA

Abstract: Thermosetting polymers comprise a wide variety of monomer constituents and polymerization chemistries that in principle provide the degrees of freedom necessary to tailor these materials to a broad range of applications, from structural composites, coatings and barrier materials, ballistic shielding, and even solid rocket fuels. In this talk, I will trace my group's history in using molecular dynamics simulations to investigate conceptual links among molecular architectures, intermolecular interactions, and network structures and how they determine themomechanical properties of polymerized materials that these applications demand. Highlights in this history include the discovery of the links between crosslink arrangements and protovoid-based toughening; toughening using partially reacted substructures; long-time-scale material response through time-temperature superposition; and rationalizing improvements over petrochemically derived monomers using novel bio-based subunits. A consistent theme will be demonstration of how close collaboration with experimental groups allows for simulation predictions to be tested. I will conclude with a presentation of our group's software package, HTPolyNet, that represents the first open-source, end-to-end generator of all-atom models of network-polymerized monomer mixtures based only on monomer structures, which should accelerate the community's use of MD simulation to investigate thermosetting polymers.



Biography: Cameron F. Abrams is the Bartlett '81 - Barry '81 Professor of Chemical and Biological Engineering at Drexel University, where he has served on the faculty since 2002 and as Department Head since 2017. Abrams' research expertise lies in advancing modern molecular simulation methods with applications in protein science, drug discovery, complex fluids, and high-performance materials. He is the recipient of an ONR Young Investigator Award, an NSF CAREER Award, and the AIChE Computational and Molecular Sciences Forum Impact Award. He received a BS in Chemical Engineering from North Carolina State University in 1995 and a PhD from the University of California, Berkeley, in 2000. He trained as a postdoc for two years in the Theory Group at the Max-Planck-Institute for Polymer Research in Mainz, Germany, before joining Drexel.