Materials Science and Engineering Department

Winter Seminar Series

Unified Particle and Field-theoretic Simulations of Polymers

Prof. Joshua Lequieu
Department of Chemical and Biological Engineering
Drexel University

February 18, 2026
11AM-12PM | Hill Seminar Room (LeBow 240)

Polymers are ubiquitous in both synthetic and biological materials and underlie technologies as diverse as surfactants, adhesives, proteins and DNA. One of the defining features of all polymeric materials is that they are characterized by a wide range of length scales, often spanning nanometers to microns. This hierarchy of length scales presents significant challenges for polymeric simulations. In this talk, I describe recent efforts by my group to develop new simulations of polymeric materials that can link monomeric to mesoscopic length scales. In the first part of the talk, I describe a new "multi-representation" simulation method where particle-based and field-theoretic simulations are linked together into a unified framework. This approach can accelerate polymer simulations by several orders of magnitude and can rapidly equilibrate mesoscopic length scales while preserving monomer-scale details and dynamics. Notably, this multi-representation approach leverages the formal equivalence between particle and field-based models and involves no approximation. The utility of this approach is illustrated by examining the self-assembly of complex sphere phases in block copolymer melts. In the second part of the talk, I demonstrate how these multi-representation simulations can be extended to explain the phase separation of biomolecular condensates. Our approach can model proteins at amino acid resolution yet is efficient enough to access the long length and time scales that characterize condensate formation. Our approach can recapitulate recent experimental data on intrinsically-disordered polypeptides and can resolve how subtle modifications to the amino acid sequence can modulate their phase behavior. Finally, we examine the phase separation of chromatin and how post-translational modifications to histone proteins can lead to transitions between liquid-like and solid-like behavior. Taken together, this work demonstrates that multi-representation simulations that combine particle and field-theoretic simulations can unlock new insights into the multiscale physics that characterize synthetic and biological polymers.

Joshua Lequieu is an Assistant Professor of Chemical and Biological Engineering at Drexel University. His research is focused on the theory and simulation of polymers and biological macromolecules such as proteins and DNA. He received a B.S. in Chemical Engineering from Cornell University and a Ph.D. in Molecular Engineering from the University of Chicago. Following a postdoc in the Materials Research Lab at the University of California, Santa Barbara, he joined Drexel University in 2020. He is the recipient of the NSF CAREER Award, the Charles E. Kaufman Foundation New Investigator Award, the Edward J. Kramer Prize in Materials and an Outstanding Teaching Award from Drexel University.
.

DREXEL UNIVERSITY
College of
Engineering

FOR MORE INFORMATION

Contact: Dr. Caroline Schauer, cls52@drexel.edu
Keiko Nakazawa, kn52@drexel.edu
drexel.edu/materials