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Coarse-grained simulations of functional copolymers

Antonia Statt—Assistant Professor, Materials Science & Engineering,
The Grainger College of Engineering, University of Illinois at Urbana-
Champaign

Abstract: In this talk, I will present two stories where coarse-grained modeling of copolymers have allowed us detailed insights into chain conformations and resulting materials behavior. The first story highlights the importance of polymer conformations and nano-scale morphology for force-responsive copolymers, where we investigate the impact of network topology on mechanochemical activation in self-assembled triblock copolymers. We find that activation during tensile deformation depends strongly on both the polymer composition and chain conformation in these materials, with activation requiring higher stress in materials with a higher glassy block content, and most activation occurring in the tie chains connecting different glassy domains.

The second story investigates the phase separation behavior of different sequences of a coarse-grained model for intrinsically disordered proteins or sequence defined block copolymers. They exhibit a surprisingly rich phase behavior, and not only conventional liquid-liquid phase separation is observed, but also reentrant phase behavior, in which the liquid phase density decreases at lower temperatures. Most sequences form open phases consisting of aggregates, rather than a normal liquid. These aggregates had overall lower densities than the conventional liquid phases and complex geometries with large interconnected string-like or membrane-like clusters. Minor alterations in the sequence may lead to large changes in the overall phase behavior, a fact of significant potential relevance for biology and for designing self-assembled structures using block copolymers. I will also discuss recent results from unsupervised manifold learning to classify the different aggregate types and what we can learn from machine learning.

Biography: Antonia Statt is an Assistant Professor in the Materials Science and Engineering Department at the University of Illinois in Urbana-Champaign since November 2019. Prior to that, she was a postdoctoral fellow at the Princeton Center for Complex Materials, where she worked in the lab of Prof. Athanassios Z. Panagiotopoulos in the CBE Department. She obtained her PhD in the lab of Prof. Kurt Binder in Physics at the University of Mainz in Germany. Her research is focused on utilizing coarse-grained computational models to further the fundamental understanding of soft matter for applications in energy and medicine. Of special interest are non-equilibrium phenomena like deformation, evaporation, and flow, as well as self-assembly and phase transitions. She received a number of Awards for her PhD work, as well as the ACS PRF young faculty Award.