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A Top Down Approach to Multiscale Modeling of Structured Materials

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There is considerable interest in developing multiscale modeling approaches capable of describing both the structure and dynamics of inhomogeneous materials having characteristic features ranging from a few to a several hundred nanometers. Examples include block polymers, which exhibit an array of ordered morphologies with characteristic dimensions in the tens of nanometers, or liquid crystalline materials, where ordered domains and defects can also span tens of nanometers. This presentation will describe a relatively new class of particle-based methods that rely on established continuum models to describe thermodynamic properties, but that adopt a molecular representation to describe molecular structure and mesoscale morphology. While these methods can describe mesoscale structure quantitatively, they can also be augmented to describe the dynamics of complex fluids, including entangled polymers, composites, and nanoparticle dispersed in structured fluids, over dynamic ranges that in some cases span multiple orders of magnitude.