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Multiscale modeling of self-assembling polymer solutions DMITRY BEDROV, Department of Materials Science & Engineering, University of Utah, GRANT SMITH, Dept. of Materials Sci. & Eng., University of Utah, BEN HANSON, Dept. of Chem. Eng., University of Utah — We have applied a multiscale modeling approach to study complex self-assembling systems such as micellar solutions and biopolymer networks. In our multiscale modeling approach we start with quantum chemistry calculations to parameterize accurate fully atomistic force fields, perform extensive atomistic explicit solvent molecular dynamics simulations on model self-assembling building blocks in solutions to understand structure and thermodynamics at atomistic scale, parameterize coarse-grained implicit solvent models, conduct extensive implicit solvent model simulations to study the self-assembly, and use a self consistent field approach to predict the system morphology. Specifically, we applied this methodology to self-assembly of triblock (PEO-PPO-PEO, Pluronic) micelles as well as to network formation of polypeptide (leucine)-modified hyaluronic acid in aqueous solutions.

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