Systematic and Simulation-Free Coarse Graining of Multicomponent Polymeric Systems

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Coarse-grained (CG) models are currently needed to simulate polymeric systems, as full atomistic simulations of many-chain systems used in experiments are in most cases not feasible due to their formidable computational requirements. Polymeric systems are also best suited for coarse graining, as the large number of monomers on each chain allows high levels of coarse graining. In this talk we will present our recently proposed systematic and simulation-free strategy for coarse graining multicomponent polymeric systems, where we use the well-developed Polymer Reference Interaction Site Model (PRISM) theory, instead of the commonly used many-chain molecular simulations, for both the original and CG systems, and examine how the CG potentials vary with the coarse-graining level and how well the CG models at various coarse-graining levels reproduce the structural and thermodynamic properties of the original system. Our strategy is quite general and versatile. It is at least several orders of magnitude faster than those using many-chain simulations, thus effectively solving the transferability problem in coarse graining, and avoids the problems caused by finite-size effects and statistical uncertainties in many-chain simulations. As examples, we have applied our strategy to the structure-based and relative-entropy-based coarse graining of homopolymers[1,2], binary polymer blends[3], and diblock copolymers in the melt state.