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Systematic and Simulation-Free Coarse Graining of Polymers QIANG WANG, Colorado State University — Coarse-grained (CG) models are currently needed to study 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. Here we introduce a systematic and simulation-free strategy for coarse graining polymeric systems, and apply it to the structure-based and relative-entropy-based coarse graining of homopolymers, polymer blends, and diblock copolymers in the melt state. We use the well-developed polymer reference interaction site model theory, instead of 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 different levels can reproduce the structure 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. It also avoids the problems caused by finite-size effects and statistical uncertainties in many-chain simulations commonly used in coarse graining.

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