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Systematic and Simulation-Free Coarse Graining of Polymer Blends QIANG WANG, Colorado State University — Here we extend our recently proposed systematic and simulation-free strategy [*D. Yang and Q. Wang*, J. Chem. Phys. **142**, 054905 (2015)] to the structure-based coarse graining of binary polymer blends. We use the well-developed polymer reference interaction site model theory, instead of many-chain molecular simulations, for both the original and coarse-grained (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 thermodynamic properties of the original system. Our strategy is at least several orders of magnitude faster than those using many-chain simulations (thus effectively solving the transferability problem in coarse graining), avoids the problems caused by finite-size effects and statistical uncertainties in many-chain simulations commonly used in coarse graining, and does not change the spinodal curve (thus also the critical point) of the polymer blends. The structure-based coarse graining, however, does not give thermodynamic consistency (i.e., the same interchain internal energy per chain or virial pressure) between the original and CG systems at any level of coarse graining.

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