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Systematic and Simulation-Free Coarse Graining of Polymeric Systems: A Structure-based Study DELIAN YANG, QIANG WANG, Colorado State University — We propose a systematic and simulation-free strategy for coarse graining of multicomponent polymeric systems, where we use the Polymer Reference Interaction Site Model theory, instead of many-chain molecular simulations, to calculate the structure and thermodynamic properties of both the original and coarse-grained (CG) models, and quantitatively examine how the effective CG pair potentials and properties of CG systems vary with the coarse-graining level. Our strategy is general and versatile, is much faster than those using many-chain simulations, and practically solves the transferability problem of coarse graining. As an example, here we apply it to structure-based coarse graining of homopolymer melts, which matches the structure correlations of CG segments between the original and CG systems. Our numerical results clearly show that structure-based coarse graining cannot give thermodynamic consistency between the original and CG systems at any coarse-graining level due to the information loss of coarse graining.

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