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Systematic and Simulation-Free Coarse-Graining of Polymer Melts using Soft Potentials DELIAN YANG, QIANG WANG, Colorado State University — Full atomistic simulations of multi-chain systems are not feasible at present due to their formidable computational requirements. Molecular simulations with coarse-grained models have to be used instead, where each segment represents, for example, the center-of-mass of a group of atoms or real monomers. While atoms interact with hard excluded-volume interactions (e.g., the Lennard-Jones potential) and cannot overlap, the coarse-grained segments can certainly overlap and should therefore interact with soft potentials that allow complete particle overlapping. Coarse-grained models, however, reduce the chain conformational entropy, which plays an essential role in the behavior of polymeric systems. In this work, we use integral-equation theories, instead of molecular simulations, to perform both the structure-based and relative-entropy-based coarse-graining of homopolymer melts, and systematically examine how the coarse-grained soft potential varies with N (the number of segments on each chain) and how well the coarse-grained models reproduce both the structural and thermodynamic properties of the original system. This provides us with a quantitative basis for choosing small N-values that can still capture the chain conformational entropy, a characteristics of polymers.

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