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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 many-chain systems such as polymer melts are not feasible at present due to their formidable computational requirements. Coarse-grained models have to be used instead, where the segments interact with soft potentials that allow complete overlapping. This enables systematic coarse-graining with different N (number of segments on each chain) at constant invariant degree of polymerization controlling the system fluctuations. In this work we use integral-equation theories and a relative entropy framework for coarse-graining to investigate how the soft potential varies with N and how well the coarse-grained models can reproduce both structural and thermodynamic properties of the original system. This will provide 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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