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Systematic and Simulation-Free Coarse Graining of Polymeric Systems: A Relative-Entropy-based Study QIANG WANG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University — Relative-entropy-based coarse graining minimizes the relative entropy (RE) quantifying the information loss due to coarse graining.[1] When pair potentials are used for coarse-grained (CG) segments, RE-based coarse graining becomes equivalent to structure-based coarse graining if the pair potentials are unconstrained.[1] Here we apply our systematic and simulation-free strategy to RE-based coarse graining of homopolymer melts; that is, we use the Polymer Reference Interaction Site Model (PRISM) theory, instead of many-chain molecular simulations, to calculate the structure and thermodynamic properties of both the original and CG systems, and quantitatively examine how the CG pair potentials and properties of CG systems vary with the coarse-graining level. We consider various analytic functional forms of CG pair potential as suggested by structure-based coarse graining, and minimize RE to obtain the associated parameters. Values of minimized RE are then used to select the appropriate analytic form of CG pair potential, which is much easier to use than the tabulated (numerical) CG pair potential obtained from structure-based coarse graining. This is the first application of RE-based coarse graining to polymers. [1] M. S. Shell, **J. Chem. Phys. 129**, 144108 (2008).

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