

Coarse-Graining of Atomistic Simulations of Polymeric Melts to Access Long Length and Time Scales

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Multiscale models of supra-molecular structure require the implementation of effective interactions between pseudo-atoms averaged over representative conformations of molecular groups. Frequently the connection between these effective interactions and the atomic identity of the molecule of interest is tenuous, and the potentials are optimized to reproduce bulk properties such as the isothermal compressibility. We present a new methodology that systematically maps the interparticle correlations from atomically detailed simulations to mesoscale potentials. The coarse-grained interactions are employed to extend simulations of oligomeric melts to characterize the structure of truly polymeric entities. The potentials determined from the present methodology can also be implemented within dissipative particle dynamic simulations to examine the dynamic properties of polymer melts.