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Representation of Polymer melts as liquids of soft-colloid chains[1]

ANTHONY CLARK, MARINA GUENZA, University of Oregon — Descriptions at various levels of coarse-graining are of great interest in understanding the complex structure and dynamics of polymer liquids, as relevant processes take place at a wide variety of length and time scales. In this talk we present a theory for a set of effective interaction potentials that map a polymer melt onto a liquid of soft-colloid chains, with each soft colloid representing the center of mass of a large subsection of a polymer chain. Molecular dynamics simulations using the effective potentials are shown to reproduce the predicted static structure, which has previously been tested against microscopic simulations. Because the theory provides analytical results and is based in first principles liquid state integral equation theory, the thermodynamics of the coarse-grained system using the effective potentials can be shown to agree with the thermodynamics of monomer-level descriptions across a range of thermodynamic states. The theory thus is able to represent of both the long-range structure and thermodynamic state of the system while retaining many-body physics on a range of large submolecular length scales.

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