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Representation of Polymer melts as soft liquids with effective pair interactions 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 and analytically characterize effective interaction potentials to map a polymer melt onto a liquid of soft spheres or soft-colloid chains, with each soft colloid representing the center of mass of a chain or large subsection of a chain. 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 scaling of the effective pair potentials beyond the physical extent of the polymer with increasing chain interpenetration is shown to be essential to capturing the contribution to the thermodynamics of the melt due to many-polymer interactions in the soft coarse-grained description, despite its vanishingly small effect on structural correlations. Further development of the theory will consider its extension from soft-colloid chains to lower level bead and spring level descriptions with the aim of gaining insight into the thermodynamic properties of these widely used models.

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