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Analytical course-grained description of a homopolymer melt as a liquid of soft colloidal chains ANTHONY J. CLARK, M.G. GUENZA, University of Oregon — Microscopic computer simulations of fluids of long polymers are greatly restricted by the limits of current computational power, and so course-grained descriptions accurate on molecular length scales are essential to extending the range of accessible systems. For some phenomena, particularly dynamical entanglement, descriptions that eliminate all internal degrees of freedom from the polymers are too drastic, as intermediate wavelength degrees of freedom are essential to the effect. Employing first-principles liquid state theory, we have developed a course-grained model for the intermolecular structure of melts of long homopolymer chains that maps each chain of hard-sphere monomers onto a chain of connected soft colloids. All dependence on system parameters is analytically expressed, so the results may be immediately applied to melts with different polymer and thermodynamic properties to calculate effective potentials between the soft-colloids on the chains, which can then be used to perform molecular dynamics simulations. These simulations capture the large wavelength structure of the system at greatly reduced computational cost, while still retaining enough internal degrees of freedom explicitly to describe phenomena that occur on length scales much larger than the monomeric units that comprise the chain, but shorter than the size of the molecule.

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