

Abstract Submitted  
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**Theoretical Multiblock Coarse-graining Approach for Homopolymer Melts** TREVOR KEIBER, University of Oregon — A microscopic theory for coarse-graining homopolymer melts as an ensemble of connected soft-colloidal particles (blocks) has been developed, which effectively maps a polymer with many monomers to a chain of soft-core bound particles. The Ornstein-Zernike liquid-state integral equation was solved to provide a mesoscopic description of the system at the level of the block centers of mass. Analytical expressions for the intramolecular and intermolecular correlation functions were derived for an arbitrary number of blocks. The block-block correlation functions were used to derive the necessary intermolecular and intramolecular coarse-grained potentials for mesoscale computer simulations.

Trevor Keiber  
University of Oregon

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