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Analytical Coarse-Grained Description of Polymer Melts and Blends EDWARD SAMBRISKI, GALINA YATSENKO, MARIA NEMIROVSKAYA, MARINA GUENZA, University of Oregon — We present an analytical coarse-grained description that maps polymer melts and blends onto fluids of soft colloidal particles. From liquid state theory, we derive the center-of-mass total pair correlation functions, $h(r)$, and the effective pair potentials, $v(r)$. The $v(r)$ serve as input to mesoscale simulations where polymer fluids are modeled as interacting soft colloidal particles. The $h(r)$ from theory and mesoscale simulations agree with united-atom simulation results with no need for fitting parameters. In this way, our approach accurately bridges between microscopic and mesoscopic descriptions of the polymer fluid structure.

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