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Simulations of polymer melts modeled as chains of interacting soft-colloids ANTHONY CLARK, MARINA GUENZA, University of Oregon — The range of time and length scales accessible to dynamical simulations of melts of long polymer chains is strongly limited by the computational demands of calculating large numbers of forces between monomers. Simulations modeling each polymer as a point particle interacting by an analytical soft pair potential have previously been successfully developed to extend this range. For many effects in polymer systems, however, submolecular degrees of freedom remain relevent to molecular-level behavior even at long times and large length scales. To allow for the inclusion of relevant submolecular degrees of freedom, we use analytical effective potentials based on our model of the structure of polymer melts on the level of large chain sub-blocks to simulate homopolymer melts. We demonstrate that structure on the block and center of mass level consistent with the structural model and monomer-level simulation data can be reproduced for large systems and long times at much lower computational cost than monomer-level simulations. Using this model, we also test the effects of additional short-range repulsive interactions between chain subunits on structure and dynamics.

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