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Theoretical Reconstruction of Realistic Dynamics of Polymer Melts from Soft Sphere Representation IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — A theoretical method to reconstruct realistic dynamics of polymer melts from highly coarse-grained descriptions has been developed from a first-principle approach. Starting from the Liouville equation and exploiting the Mori-Zwanzig projection operator formalism we have derived the generalized Langevin equations for the coarse-grained representations of polymer melts. Each polymer chain is coarse-grained at two levels: at the monomer level and at the molecular level as a soft sphere. By enforcing equivalence between the two descriptions in the long time regime where the internal dynamics is completely relaxed we derived an analytical rescaling formalism. Change in entropy and change in friction are the two corrections that need to be accounted. The rescaling factors explicitly depend on the thermodynamic and molecular parameters of the system simulated. After applying our reconstruction method, the dynamics obtained from mesoscale simulations of polyethylene and polybutadiene, represented as soft-colloidal particles, show quantitative agreement with experiments and atomistic simulations. The predictive power of the method is demonstrated for samples of long polyethylene chains.

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