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Coarse-Graining of Polymer Dynamics via Energy Renormalization WENJIE XIA, National Institute of Standards and Technology, JAKE SONG, Northwestern University, FREDERICK PHELAN, JACK DOUGLAS, National Institute of Standards and Technology, SINAN KETEN, Northwestern University —
The computational prediction of the properties of polymeric materials to serve the needs of materials design and prediction of their performance is a grand challenge due to the prohibitive computational times of all-atomistic (AA) simulations. Coarse-grained (CG) modeling is an essential strategy for making progress on this problem. While there has been intense activity in this area, effective methods of coarse-graining have been slow to develop. Our approach to this fundamental problem starts from the observation that integrating out degrees of freedom of the AA model leads to a strong modification of the configurational entropy and cohesive interaction. Based on this observation, we propose a temperature-dependent systematic renormalization of the cohesive interaction in the CG modeling to recover the thermodynamic modifications in the system and the dynamics of the AA model. Here, we show that this energy renormalization approach to CG can faithfully estimate the diffusive, segmental and glassy dynamics of the AA model over a large temperature range spanning from the Arrhenius melt to the non-equilibrium glassy states. Our proposed CG strategy offers a promising strategy for developing thermodynamically consistent CG models with temperature transferability.

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