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Abstract for an Invited Paper for the MAR15 Meeting of the American Physical Society

Thermodynamically Consistent Coarse-Graining of Polymers¹

MARINA GUENZA, University of Oregon

Structural and dynamical properties of macromolecular liquids, melts and mixtures, bridge an extensive range of lengthand time-scales. For these systems, the computational limitations of the atomistic description prevent the study of the properties of interest and coarse-grained models remain the only viable approach. In coarse-grained models, structural and thermodynamic consistency across multiple length scales is essential for the predictive role of multi-scale modeling and molecular dynamic simulations that use mesoscale descriptions. This talk presents a coarse-graining approach that conserves structural and thermodynamic quantities independent of the extent of coarse-graining, and describes a model for the reconstruction of the dynamics measured in mesoscale simulations of the coarse-grained system. Some of the general challenges of preserving structural and thermodynamic consistency in coarse-grained models are discussed together with the conditions by which the problem is lessened.

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