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Solvent Entropy in and Coarse-Graining of Polymer Lattice Models QIANG WANG, PENGFEI ZHANG, Department of Chemical and Biological Engineering, Colorado State University — In conventional lattice models for polymeric systems, each lattice site is occupied by at most one polymer segment, and an unoccupied lattice site is often treated as a solvent molecule. This self- and mutual-avoiding walk requires that all lattice sites, polymer segments, and solvent molecules have the same volume. Since a polymer segment here is the coarse-grained representation of a group of real monomers, this incorrectly accounts for the solvent entropy (i.e., size ratio between polymer segments and solvent molecules). It also limits the coarse-graining capability of such models, where the invariant degree of polymerization controlling the system fluctuations is too small (thus exaggerating the fluctuations) compared to that in most experiments. Here we show how to properly account for the solvent entropy in new lattice models with multiple occupancy of lattice sites [Q. Wang, **Soft Matter 5**, 4564 (2009); **6**, 6206 (2010)], and present a quantitative coarse-graining strategy that ensures both the solvent entropy and fluctuations in experimental systems are properly accounted for using the new lattice models.

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