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Minimal Energy Polymer Packings[1]

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We examine the structure and dynamics of collapsed polymers using a variety of simulation and theoretical techniques. For flexible chains of N "sticky" tangent hard spheres, at small N, the ground states are the same as for the nonpolymeric case (NPC) [1], while at large N the ground states are crystallites with close-packed cores. The polymeric nature of the packings gives rise to distinguishable ground-state structures whose multiplicity relative to the NPC grows rapidly with N. We explicitly enumerate the polymer packings for small N and study the most likely packings for large N. We explore the extent to which the packing types and probabilities change with several important properties of the polymer, including the softness of the interaction potential, bending stiffness, bond length, and heterogeneity of the monomers. Typically, small variations of these properties break the degeneracy of NPC ground states, while large variations produce qualitatively different ground-state packings. We also characterize the slow dynamics of transitions between low-energy states at finite temperature.

[1] N. Arkus, V. N. Manoharan, and M. P. Brenner, PRL, 103, 118303 (2009).

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