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The relation between collapsed states of a polymer chain and compact Lennard-Jones clusters¹ KATJA SCHAEFER, M. A. NOVOTNY, Department of Physics and Astronomy, Mississippi State University, C. S. O'HERN, Department of Mechanical Engineering and Department of Physics, Yale University — We present computational studies of compact states of small linear polymer chains consisting of hydrophobic and polar monomers. At sufficiently low temperatures, the polymer chain undergoes a transition from a fully extended to a compact state, and the dynamics of the collapse process is studied with a particular emphasis on the distribution of the end-to-end distances of the polymer. We show that in certain parameter regimes the distribution of end-to-end distances of the polymer chain near the ground state resembles the distribution of the pairwise distances of compact Lennard-Jones (non-polymeric) clusters.

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