

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

An off-lattice Wang-Landau simulation of the coil-globule and solid-liquid transitions of flexible homopolymers. DREW PARSONS, DAVID WILLIAMS, Australian National University — The temperature-independent Wang-Landau Monte Carlo approach is implemented for an off-lattice model of flexible homopolymers and applied to the study of the coil-globule and solidification transitions. Transition temperatures are calculated and the thermodynamic limit of the two transitions is compared. We address the issue of obtaining crystal structure in the low energy solid globules, and raise the question of whether a glass-like state rather than crystalline is a correct description of the solid state.

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Date submitted: 11 Jan 2006

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