419e Density-of-States Simulation of Collapse of Confined Heteropolymers

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The Wang-Landau Monte Carlo method of direct density-of-states calculation has been adapted for off-lattice simulation of mechanical confinement of a generic multiblock-copolymer undergoing a first-order folding transition. We developed a novel suite of trial moves, including a ``partial NVE MD'' move. Using this technique we have quantified the increase in thermal stability of a native ``folded'' state in a spherical confining geometry, measured as an increase in melting temperature with decreasing radius of the confining sphere. The degree of stabilization as a function of the confining sphere radius is shown to follow a simple scaling relationship in which the changes in the latent heat and entropies upon confinement are allowed to scale independently. It is hoped that an efficient density-of-states algorithm such as ours provides a new tool in pursuing a theoretical understanding of both the thermodynamics and kinetics of confined proteins.