Abstract Submitted
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Polymer chain folding in spherical nano-confinement[1] ANTONIA SIKON, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — Nano-scale confinement of a polymer chain results in a loss of conformational entropy. For a chain that can fold into a compact native state, such confinement reduces the number of possible unfolded configurations, thereby stabilizing the folded state and shifting the location of the folding transition. Here we investigate these confinement effects for a flexible polymer confined within a rigid sphere of diameter D. We study a square-well-sphere chain that undergoes a first-order-like folding transition analogous to the all-or-none folding characteristic of many small proteins [1]. We construct the partition function for this chain under confinement using a Wang-Landau simulation approach. The resulting temperature vs confinement length D phase diagram shows stabilization of the folded state with decreasing D and the possibility of confinement induced isothermal folding [2]. The folding transition remans first-order-like even in extreme confinement with a free energy barrier that is little affected by changes in D. [1] Taylor, Paul, and Binder, J. Chem. Phys. 145, 174903 (2016); [2] Taylor, Macromolecules 50, 6967 (2017).

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