Abstract Submitted
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All-or-none folding of a polymer in confinement[1] MARK TAYLOR, Hiram College — A flexible homopolymer chain with sufficiently short-range interactions undergoes a discontinuous transition from an expanded coil to a compact crystallite analogous to the all-or-none folding transition exhibited by fast-folding proteins. One anticipates that geometric confinement will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to higher temperature. In this work we study a flexible square-well N-mer chain (monomer diameter d) located between two hard walls forming a slit-like pore (width W) with the chain end-tethered to one wall. We carry out Monte simulations with Wang-Landau sampling to construct the single-chain density of states and use both microcanonical and canonical analyses to characterize phase transitions. When the slit width is similar to the size of the folded chain we observe a modest stabilization effect. Further reduction of the slit width geometrically prohibits the chain from folding into the free-chain ground state. However, a discontinuous all-or-none folding transition still occurs to a flattened crystallite that spans the pore. All-or-none folding persists even to the limit of a very narrow pore (W d) where the ground-state structure is a quasi-two-dimensional crystal.

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