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Polymer folding in confined and crowded environments[1] MARK TAYLOR, CHRISTOPHER VINCI, Hiram College — A single polymer chain can undergo a series of conformational transitions analogous to the phase transitions exhibited by bulk materials. We have recently studied the conformational transitions of a flexible square-well polymer chain using a Wang-Landau simulation approach in which we directly compute the single-chain partition function [1]. For the case of a tangent-sphere chain, a sufficiently short-range interaction gives a direct coil-crystal transition analogous to the all-or-none folding transition exhibited by fast-folding proteins. Here we investigate the effects of geometric confinement on this folding transition. One anticipates that confinement will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to higher temperature. Here we study the folding transition of a flexible square-well N-mer chain (monomer diameter d) that is (A) located between two hard walls forming a slit-like pore with the chain end-tethered to one wall and (B) immersed in a hard-sphere solvent with solvent diameter D >= d and solvent volume fraction 0 < vf < 0.4. An entropic stabilization effect is found in both cases. [1] Taylor, Paul, and Binder, J. Chem. Phys. 131, 114907 (2009)

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Mark Taylor
Hiram College

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