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Effects of confining a polymer chain in a cylindrical pore[1] CHRISTIAN O'NEIL, MARK TAYLOR, Dept. of Physics, Hiram College — Polymers attached to a surface can change the properties of that surface drastically. These tethered polymers can undergo conformational transitions (e.g., change between expanded, collapsed or folded shapes) that provide additional control of surface properties. Tethering polymers inside pores in a surface might provide an on/off switch between a polymer coated surface (chains expanded) and a polymer free surface (chains folded and retracted into the pores). Here we study the effects of confinement in a cylindrical pore on the phase transitions of a single polymer chain. In particular, we study the all-or-none folding transition of a 32 bead square-well-sphere chain with a short-range interaction. We carry out Monte Carlo computer simulations using the Wang-Landau algorithm to obtain the single chain density of states for this system. These results allow us to determine phase transition temperatures and thus, investigate how confinement affects phase behavior. For narrow pores we find a small entropic stabilization of the folded chain with decreasing pore diameter.

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