Abstract Submitted
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Adsorption transition for a polymer chain in a narrow slit[1] NORAH ALI, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — Here we study the adsorption of a confined flexible polymer chain to an attractive surface. The polymer is end-tethered to an attractive plane which forms one wall of a slit-like pore. At low temperature the polymer will be completely adsorbed on to the attractive wall while at high temperature the polymer will be desorbed and in a random coil configuration. We use a Wang-Landau simulation algorithm to compute the density of states of this system from which we can construct the complete thermodynamic behavior. Our main interest is how the width of the slit affects the location of the adsorbed-to-desorbed transition. Geometric confinement usually favors a compact state over an expanded state [1], however, here we find that as the slit width is decreased the desorbed (expanded) state is favored (i.e., the transition moves to lower temperature). For extremely narrow slits (where we have a pseudo 2D system) we find a crossover to stabilization of the adsorbed (compact) state. We also study the effects of chain length on the location of this transition. [1] Taylor, Macromolecules 50, 6967 (2017).

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