

Abstract Submitted
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Tethered chains in good and poor solvent - effects of lateral confinement on adsorption and chain collapse JUTTA LUETTNER-STRATHMANN, University of Akron — The grafting density of a polymer brush affects the response of the system to changes in solvent quality and surface interactions. In this work, we focus on low (mushroom) and intermediate (semi-dilute regime) grafting densities and model a polymer chain in a brush as a single tethered chain subject to an applied force field of cylindrical symmetry that pulls the chain segments toward an axis through the tethering point and normal to the surface. The polymer chain is represented by a bond-fluctuation model with extended range attractive bead-bead interactions and variable bead surface interactions. Monte Carlo simulations with a Wang-Landau type algorithm are performed to determine the density of states in the state space of monomer-monomer contacts, monomer-surface contacts, and lateral chain extension. We present results for the effect of lateral confinement on conformational transitions such as chain adsorption in good and poor solvent.

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