Transitions of tethered polymer chains JUTTA LUETTMER-STRATHMANN, University of Akron, FEDERICA RAMPF, WOLFGANG PAUL, KURT BINDER, Johannes Gutenberg Universität Mainz — Polymer chains near surfaces with attractive monomer surface interactions undergo a transition from three-dimensional to two-dimensional conformations as the temperature is lowered. In good solvent conditions, this is a well-known adsorption transition, which corresponds to a bicritical point in the infinite chain limit; it is continuous and the adsorption temperature is independent of the (net) interaction strength between monomers. In poor solvent, on the other hand, the transition is not well understood. In this work, we present simulation results for a flexible lattice model of a single chain tethered to a surface. A two-dimensional Wang- Landau algorithm was employed to obtain a density of states in the space of surface and monomer-monomer contacts for several chain lengths. The density of states was evaluated with interaction parameters spanning the range from good to poor solvent conditions and from repulsive to strongly attractive surfaces. Our results for good-solvent conditions show the expected adsorption transition. In poor solvent, we find a splitting of the adsorption transition into two main branches, which may be interpreted in terms of a drying and wetting transition, where the wetting transition proceeds through a series of layering transitions.

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