Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage

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We analyze the adsorption propensity of a single polymer confined in a spherical cage with attractive walls [1,2]. The polymer is modeled in a coarse-grained continuum formulation by 12-6 Lennard-Jones interactions among the monomers and a very weak bending energy. By means of extensive parallel tempering and multicanonical Monte Carlo simulations it is shown that the system exhibits a rich phase diagram in the adsorption strength-temperature plane, ranging from highly ordered, compact to extended, random coil structures and from desorbed to partially or even completely adsorbed conformations. These findings are identified by canonical and microcanonical analyses techniques using different energetic and structural observables such as the gyration tensor and universal shape parameters that characterize the asphericity of a typical polymer conformation. The talk concludes with a discussion of the similarities and differences to a polymer adsorbing to a solid attractive substrate [3] or to a fluctuating attractive membrane [4], allowing for a back-reaction of polymer and substrate degrees-of-freedom.

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