

Computer Simulation Studies of Polymer Adsorption and Aggregation

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The talk gives an overview on our recent computer simulation studies of polymer adsorption and aggregation using generic coarse-grained models. The simulations are performed with Monte Carlo methods in generalized ensembles (multicanonical and parallel tempering) and analyzed from a canonical and microcanonical view. The adsorption properties are discussed for polymer chains interacting with a flat patterned surface or being confined in a spherical cage. Special emphasis will be given to the scaling properties of conformational transitions in dependence of the polymer's bending stiffness. Bending stiffness also plays a key role for semiflexible polymer aggregation. Our recent results show that this is the distinguishing parameter that controls whether amorphous aggregates or twisted bundle-like motifs are formed.