

Abstract Submitted
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Weak polyelectrolytes grafted to nanoparticles and flat surfaces

STEPHEN BARR, ATHANASSIOS PANAGIOTOPOULOS, Chemical and Biological Engineering, Princeton University — The charge distribution on polyelectrolytes is a key factor which controls their conformation and interactions. In weak polyelectrolytes, this distribution is determined by a number of factors, including the solvent conditions and the local environment. We investigate this using grand canonical titration Monte Carlo simulations of a coarse grained polymer model. In this method, each polymer bead is able to change its ionization state based on its dissociation constant, the pH of the solution, and interactions with other particles in the system. We focus on a system of polymers with one end tethered to the surface of a nanoparticle and determine both the charge and the polymer conformation as the pH and solvent quality are varied. We compare the results to both a fixed charge model and to polyelectrolytes grafted to a flat surface.

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