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Sequence effects on Polyelectrolyte Complexation[1] MICHAEL MCGOVERN, DAVID MORSE, KEVIN DORFMAN, University of Minnesota — The complexation of a polyelectrolyte with an oppositely charged micelle is an important problem, with particular applications in the formulation of materials such as gene delivery vehicles. The physical process driving complexation is complicated, involving both counter-ion release and redistribution of charge inside the micelle. Recent experiments indicate that both the thermodynamics and the dynamics of this process are affected by the charge sequence of the polyelectrolyte. Motivated by these experiments, we have performed molecular dynamics simulations on the complexation between free polyelectrolytes in solution and an oppositely charged polyelectrolyte brush, serving as a simple model for a micelle. One of the moieties is a polyelectrolyte with uniform change density and the other is a copolymer. We consider different types of copolymers (block, alternating) to address the effect of charge sequence. We will present results on the effects of sequence on chain mobility, the frequency of exchanges between bound and free polyelectrolytes, and the degree of overcharging of the complexes under different conditions of polyelectrolyte concentration and salt concentration.

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