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Molecular Dynamics Simulations of Polyelectrolyte Adsorption at Oppositely Charged Surfaces JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — We have performed molecular dynamics simulations of polyelectrolyte adsorption at oppositely charged surface from dilute polyelectrolyte solutions. In our simulations polyelectrolytes are modeled by chains of charged Lennard-Jones particles with explicit counterions. We have studied the effects of surface charge density, surface charge distribution, solvent quality for the polymer backbone, strength of the electrostatic and short-range interactions on the polymer surface coverage and thickness of the adsorbed layer. We have observed surface undercharging by adsorbing polyelectrolyte in most systems except for systems with low surface charge densities. This undercharging is due to partial screening of the surface charge by surface counterions however this effect is negligible at low surface charge densities. Surface overcharging was also observed for the so-called "salt-free" systems in which only counterions necessary for neutralization of the charge difference between surface charge and polyelectrolytes were kept in the system. Hydrophobic polyelectrolytes cover higher percentage of the adsorbing surface forming a thinner polymeric layer in comparison with those observed in the systems with hydrophilic polyelectrolytes. However, the polymer surface coverage is close for both these systems.

Andrey Dobrynin
University of Connecticut

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