141g Density Functional Theory for Polyelectrolytes near a Charged Surface

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There has been growing interest recently to study the adsorption of polyelectrolytes at surface due to its close relevance to biological systems. In this work, we present a new density functional theory for the configuration of coarse-grained polyelectrolytes near a charged surface following a restrictive primitive model where the counterions and co-ions are represented by charged hard spheres of equal size and the solvent is represented by a dielectric medium. By an extensive comparison with the simulation results, we find that the agreement between theoretical predictions and simulation data is excellent at a variety of solution conditions including valence, solution concentration and surface charge density. Different from previous theoretical approaches based on the Poisson-Boltzmann equation, self-consistent-field theory or alternative density-functional theories, the new theory is also able to capture the layering and charge inversion effects.