518g Strong Charge Inversion and Layer-by-Layer Assembly of Flexible Polyelectrolytes from Self-Consistent Field Calculations

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We have applied a self-consistent field theory (SCFT) to flexible polyelectrolytes (PE) on flat surfaces either uncharged or carrying opposite charges to the PE. We examined in detail the effects of various parameters on PE adsorption and surface charge compensation by the adsorbed PE. The ground-state dominance approximation (GSDA) was used to explore the large parameter space involved, including the charge distribution and degree of ionization of PE, surface charge density, short-range (non-Coulombic) surface-polymer interactions, solvent quality, bulk polymer concentration and salt concentration. The results from GSDA were also compared with those from full SCFT calculations to examine the effects of molecular weight of PE. Strong charge inversion is found for long PE on oppositely charged, attractive surfaces in poor solvent at high salt concentrations.

We further modelled the process of layer-by-layer assembly of flexible PE using the mean-field theory, to examine the layer thickness and internal structure of the PE multilayer. Our results agree with most experimental findings on the PE layer-by-layer assembly process. Further work on exploring the importance of correlations and fluctuations in the system is undergoing.