Self-Consistent Field Calculations of Polyelectrolytes on Flat Surfaces QIANG WANG, Colorado State University, GLENN FREDRICKSON, University of California-Santa Barbara — We apply a self-consistent field (SCF) theory to study the behavior of polyelectrolytes (PE) on flat surfaces either electrically neutral or carrying opposite charges to the PE. In the former case, PE are less depleted from a non-adsorbing surface than neutral polymers, due to the presence of counterions near the surface. In the latter case, PE form an adsorption layer near the surface (with no salt added). We then compare the results from full SCF calculations with those obtained under the ground state dominance approximation (GSDA); our results show that the GSDA gives in most cases good quantitative description for PE adsorption on oppositely charged surfaces. Finally, we examine in detail the effects of various parameters on PE adsorption and surface charge compensation by the adsorbed PE, including the charge distribution and degree of ionization of PE, surface charge density, short-range interactions between the surface and polymer, solvent quality, bulk polymer concentration and salt concentration. Our results show that, for PE on oppositely charged surfaces, Coulombic interactions dominate in most cases with no added salt. In such cases, adsorbed PE almost exactly compensate the surface charge; the bulk polymer concentration, solvent quality, and short-range interactions between the surface and polymer have little effects on the amount of adsorbed PE. The added salt plays an important role by screening Coulombic interactions. Further work exploring the importance of fluctuations in the system is undergoing.

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