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**Charge regulation and local dielectric function in planar polyelectrolyte brushes** RAJEEV KUMAR, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831, BOBBY SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831, S. MICHAEL KILBEY II, Department of Chemistry, University of Tennessee, Knoxville, TN-37996 & Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Understanding the effect of inhomogeneity on the charge regulation and dielectric properties, and how it depends on the conformational characteristics of the macromolecules is a long-standing problem. In order to address this problem, we have developed a field-theory (J. Chem. Phys. 136, 234901 (2012)) to study charge regulation and local dielectric function in planar polyelectrolyte brushes. The theory is used to study a polyacid brush in equilibrium with a bulk solution containing monovalent salt ions, solvent molecules, and pH controlling acid. In particular, we focus on the effects of the concentration of added salt and pH of the bulk in determining the local charge and dielectric function. Our theoretical investigations reveal that the dipole moment of the ion-pairs formed as a result of counterion adsorption on the chain backbones play a key role in affecting the local dielectric function. Furthermore, an increase in the bulk salt concentration is shown to increase the local charge inside the brush region.

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