

Abstract Submitted
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Polyelectrolyte complexes and salt: a computational study

HANNE ANTILA, Aalto University, Department of Chemistry, PAUL VAN TASSEL, Yale University, Chemical and Environmental Engineering, MARIA SAMMALKORPI, Aalto University, Department of Chemistry — Charged polymers, polyelectrolytes (PEs), are versatile materials with applications ranging from tissue engineering to sensing elements. In aqueous solutions, oppositely charged PEs form complexes which are known to be sensitive to added salt with responses including shrinking, flocculation or swelling, and at higher concentrations loosening and destabilization of the complex. However, the role of electrostatics, charge correlations, hydration, and ion specific interactions remain unclear. In this work, we use all-atom molecular dynamics with explicit water and ions to probe the effect of excess salt to DNA-polylysine complex formation and stability, and demonstrate the mechanism of PE and ion species specific salt-driven dissociation [1]. The dissociation occurs accompanied by charge reversal in which charge correlations and ion binding chemistry play a role. Our results agree with experimental work on complex dissociation but in addition show the underlying microstructural correlations driving the behavior. We expand the full atomic level detail and dynamics results with theoretical and computational work describing the PE complex as oppositely charged rods to provide a more complete understanding of PE interactions in salt. [1] H. Antila and M. Sammalkorpi, submitted (2013)

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