

Abstract Submitted
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A molecular simulation study on salt response of polyelectrolyte complexes HANNE ANTILA, Aalto University, Department of Chemistry, PAUL VAN TASSEL, Yale University, Chemical and Environmental Engineering, MARIA SAMMALKORPI, Aalto University, Department of Chemistry — In aqueous solutions, oppositely charged polymers, polyelectrolytes (PEs) form complexes which are known to be sensitive to added salt with responses ranging from shrinking to full destabilization of the complex. As a specific application of PE complexes, the complex formation of DNA with polycations has been demonstrated to be an effective means of transfecting genetic material in gene therapy. We use all-atom molecular dynamics and coarse-grained Monte Carlo simulations to investigate the effect of excess salt on DNA-polycation complex stability. The detailed all-atom simulations demonstrate the mechanism of polycation and ion species specific salt-driven dissociation [1] involving charge reversal. More generally, other possible mechanisms of salt driven dissociation exist as well. The coarse grained approach, which describes the PE complex as oppositely charged, rigid rods and ions as hard spheres, provides a more complete understanding of PE interactions in salt, and suggests possible mechanisms leading to repulsion between the oppositely charged polyelectrolytes. [1] H. S. Antila, M. Sammalkorpi, J. Phys. Chem. B, 2014.

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