

Abstract Submitted
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Polyelectrolyte Complexes in Solution: A Molecular Dynamics Study¹ YANFEI TANG, SHENGFENG CHENG, Virginia Tech — Ion-containing polymers are important materials in food, energy, and water industry. To better understand how the structures of polyelectrolytes, we employ molecular dynamics simulations to study the complexation of oppositely charged polyelectrolyte chains in a solution. Polyelectrolytes are modeled as bead spring chains of charged Lennard-Jones (LJ) particles. Solvent is treated as a dielectric background. Explicit counterions and salt ions, treated as single LJ beads, are included in the model. Our simulations show that the structure of the resulting complex formed by polyanions (PAs) and polycations (PCs) depends on the charge ratio (x) between PC and PA chains and the salt concentration (C_s). At x near 1 and small C_s , all chains condense into a macroscopic drop. Our results show that the macroscopic drop phase exists only in a small range of C_s and is destabilized when C_s is increased. When x is smaller than 1, the number of PC chains is insufficient to neutralize all PA chains. When x is large than 1, one or several PA chains form complexes with abundant PC chains that are positively charged. Our simulations suggest that the macroscopic drop phase become unstable when x deviates from 1 in both negative and positive directions.

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