

Abstract Submitted
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Polyelectrolyte Complexes in Solution: A Molecular Dynamics Study¹ YANFEI TANG, SHENGFENG CHENG, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA — Ion-containing polymers including polyelectrolytes are important materials in food, energy, and water industry. To better understand the morphology and fabrication of polyelectrolyte based materials, we employ molecular dynamics simulations to study the complexation of oppositely charged polyelectrolyte chains in solution. Our simulations show that the structure of the resulting complex formed by polyanions (PAs) and polycations (PCs) depends on the charge ratio (x) between the PC and PA chains and salt concentration (Cs). At x near 1 and small Cs , all chains condense into a macroscopic drop. This macroscopic drop phase exists only in a small range of Cs and is destabilized when Cs is increased beyond a certain x -dependent threshold. 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 fractal-like complexes with abundant PC chains. 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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