

Molecular Dynamic Simulations of Polyelectrolyte Complexes and their Behavior at the Air-Water Interface with Variable Salt Concentrations

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The investigation of peptide-based polyelectrolyte complexes (PECs) is of great interest due to its application for the food and drug industries. These complexes emerge during phase separation wherein oppositely charged polymers are mixed in aqueous media. Previous studies by Rajpersaud *et al* investigate sequence-dependence in peptides to optimize specific material properties of the complex, such as interfacial tension and viscosity. Here, we investigate salt-dependence in peptides by reporting microsecond molecular dynamic simulations to characterize the effect of varying ion (NaCl) concentrations on the peptide conformation for model polypeptide sequences that were previously reported by Tabandeh *et al*. Standard water boxes and boxes with an air-water biphasic are generated for these analyses. The relationship between ion concentration and coacervation behavior is analyzed using its radial distribution function (RDF), radius of gyration (R_g), and solvent accessible surface area (SASA). Interfacial tension (IFT) is calculated to determine activity along the interface using pressure tensor anisotropy and mean squared displacement (MSD). This analysis makes inferences on trends in peptide conformation and salt concentration which are consistent with experimentally reported results.

Keywords: polyelectrolyte complexes, ion concentration, coacervation behavior, peptides.