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Multibody Interactions, Phase Behavior and Clustering in Nanoparticle-Polyelectrolyte Mixtures VENKATRAGHAVAN GANESAN, GUNJA PANDAV, VICTOR PRYAMITSYN, Univ of Texas, Austin, JEFFREY ERRINGTON, SUNY Buffalo — We present the results of a computational study of the interactions, phase-behavior and aggregation characteristics of charged nanoparticles (CNPs) suspended in solution of oppositely charged polyelectrolytes (PEs). We used an extension of the mean-field polymer self-consistent field theory (SCFT) model to explicitly characterize the multibody interactions in such systems. For dilute-moderate particle volume fractions, the magnitudes of three and higher multibody interactions were seen to be weak relative to the contributions from pair interactions. We embedded the pair-interaction potentials within a thermodynamic perturbation theory approach to identify the phase behavior of such systems. The results of such a framework suggested that the gas and FCC crystal phases were thermodynamically stable, whereas the fluid-like phase was metastable in such systems. To complement the parameters studied, we used a recently developed simulation approach to study the aggregation and cluster morphologies in CNP-PE mixtures. For low particle charges, such systems mainly exhibited clusters arising from direct contact aggregation between CNPs. However, for higher particle and PE charges and low PE concentrations, large regions of PE-bridged clusters were seen to form.

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