Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Mesoscale Simulations of pH-Responsive Swelling of Polyelectrolyte Complexes[1] SHIYI QIN, XIN YONG, Binghamton Univ — Using dissipative particle dynamics (DPD), we model the swelling behavior of polyelectrolyte complexes formed by two oppositely charged linear polymers while changing the ionization of cationic polyelectrolyte according to the Henderson-Hasselbalch equation. The electrostatic interactions are solved using a modified Particle-Particle-Particle-Mesh (PPPM) method, which implements an iterative Poisson solver. We characterize the formation of the complex from two separated chains and elucidate the influence of ionization of the cationic polyelectrolyte on the morphology of the complex. The radial distribution functions and the radius of gyration of each polyelectrolyte are calculated to quantify the conformational changes. We find that the complex swells and shrinks depending on the degree of ionization and subsequently correlate the swelling ratio with the pH value. We further reveal the effects of the polyelectrolyte sizes, the concentration of monovalent salts on the swelling behavior of polyelectrolyte complexes.

[1]This research supported by the American Chemical Society Petroleum Research Fund (Award 56884-DNI9)

Shiyi Qin
Binghamton Univ

Date submitted: 09 Nov 2016 Electronic form version 1.4