Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Simulation of complexes between linear polyelectrolyte and charged dendrimer GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — Complexes formed by electrostatic interactions between dendrimer having cationic terminal groups and anionic linear polyelectrolyte are studied using hybrid Monte Carlo simulations. The excluded volume interactions are modeled using a self-consistent field and the electrostatic interactions are computed by solving Poisson equation. Such framework facilitates simulating large scale three-dimensional systems. We primarily focus on the effect of dendrimer generation number, stiffness of polyelectrolyte chain and systematically study its effect on change in shape and size of complexes. Our results suggest that the dendrimer structure and charge distribution has a significant impact on the complex formation.

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Date submitted: 15 Nov 2013 Electronic form version 1.4