

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Complexation between Charged Dendrimers and Polyelectrolytes

GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — We extend the single chain in mean field simulation framework to treat charged nanoparticles in polyelectrolyte solution in presence of explicit counterions and salt. We use two models to depict nanoparticles, viz., soft nanoparticles in the form of dendrimers and hard nanoparticles having impenetrable core and penetrable outer shell. For both models, a systematic analysis of properties of complexes formed due to electrostatic interactions is carried out using radial distribution functions, charge distribution, complex size distribution, etc. In addition, we also comment on the structure of complexes formed as a function of charge on nanoparticles and polyelectrolytes.

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Date submitted: 12 Nov 2014

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