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Phase behavior and multi-body effects in polyelectrolyte - nanoparticles mixtures VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin, JEFFREY ERRINGTON, University at Buffalo — Recently we have developed a SCFT approach which allowed us to compute the effective interactions between charged nanoparticles (CNP) and in a polyelectrolyte (PE) solution. We have adapted such an approach to study the hierarchy of the two-, three- and multi-body interactions between CNP's. We have found that for the strong PE's and absent polarization interactions, the CNP-CNP interactions are essentially pairwise. This result allowed us to use the thermodynamic perturbation theory and the MC simulations to access the phase diagram of PE/CNP mixtures. Such analysis indicates that CNP-PE mixtures exhibit only gas and crystal phases, and that the fluid phase is metastable. The results of MC simulations suggest the suppression of the phase segregation by the formation of highly anisotropic clusters of CNP. The qualitative analysis of the three- and multi-body interaction in comparison with two-body interaction shows that such interaction may enhance the anisotropy of CNP clusters. We have also analyzed of weak PE's and the presence of polarization interaction. In such systems CNP's interactions remain qualitatively similar to the above systems, but the multi-body interactions appears to be significantly enhanced, which makes anisotropic clustering of PE's even more plausible.

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