Abstract Submitted
for the TSS12 Meeting of
The American Physical Society

An optimized theory for charged macroions immersed in a molecular electrolyte[1] DAMIEN VILLARREAL, ZAVEN OVANESYAN, MARCELO MARUCHO, Department of Physics and Astronomy, University of Texas at San Antonio — Widespread work in theory, experiment, and computation has been carried out to gain a fundamental understanding of the rich, yet sometimes counterintuitive, behavior of charged macroions immersed in a molecular electrolyte. Due to strong interactions with the macroion surface and with each other, screening Z-ions are not positioned randomly in 3D space, but form a strongly correlated liquid on the surface of the macroion. Hence, a detailed knowledge of the structural arrangement g(r) of ions and water molecules in the vicinity of a macroion is of crucial importance to get a microscopic understanding of polyelectrolyte systems. To achieve this, novel computational methods are required to treat the solvent effects on macroions at the atomic level. In this poster, we present an approximation optimized for integral equation theories to compute g(r) for molecular fluids. It is especially designed to take advantage and eliminate deficiencies present in old, but still used approximations, including HNC and PY. As a preliminary test, we calculate correlation functions g(r) for spherical nanoparticles immersed in an aqueous electrolyte, achieving a compromise between accuracy and computational cost without suffering the limitations demanded by full atomistic simulation calculations.

[1]NSF - PREM

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Date submitted: 15 Feb 2012 Electronic form version 1.4