Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

An Optimized Solvation Theory for Charged Macromolecules Immersed in Aqueous Electrolyte Solutions ZAVEN OVANESYAN, BHARAT MEDASANI, MARCELO MARUCHO, University of Texas at San Antonio, MONICA OLVERA DE LA CRUZ GROUP AT NORTHWESTERN UNIVERSITY COLLABORATION — In this talk, we introduce an accurate solvation model based on integral equation theory to study highly interacting charged systems. This approach is able to account for strong ion screening effects on charged macromolecules where conventional approaches may be inappropriate. A detailed knowledge of the structural arrangement of ions and solvent molecules in the vicinity of macromolecules is of crucial importance to get a microscopic understanding of these polyelectrolyte systems. We present the results obtained for ion-sphere density profiles, integrated charge and mean-electrostatic potential. These calculations are generated at low computational cost without losing important structural features of these strongly interacting charged systems. The results predict charge inversion and are in good agreement with Monte Carlo simulations.

Zaven Ovanesyan
University of Texas at San Antonio

Date submitted: 07 Nov 2012 Electronic form version 1.4