Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Nanoparticles in Aqueous Media: Crystallization and Solvation Charge Asymmetry[1] WILLIAM KUNG, Northwestern University, PEDRO GONZALES, Cinvestav del IPN, MONICA OLVERA DE LA CRUZ, Northwestern University — We examine the issue of whether dispersion forces can lead to crystallization in a system of charged nanoparticles in aqueous solution with NaCl salt. To this end, we determine the effective pair potential (EPP) among the nanoparticles, starting from a model system that explicitly includes the salt ions and the water molecules. In particular, we used the well-tested simple point charge extended (SPC/E) model for the water molecules and the reference interaction site model (RISM) equation complemented with the hypernetted-chain (HNC) closure to compute the pairwise correlations among the components. As such, we derive the phase diagram for our system using a mean-field approach based upon the computed EPP, for a range of (finite) nanoparticle densities and salt concentrations, and demonstrate crystallization. Findings from our model also suggest strong trends of charge asymmetry due to solvation effects.

[1]W. K. acknowledges the funding from the Nanoscale Science and Engineering Initiative by the National Science Foundation (NSF) under the Award Number EEC-0647560 and from NSF grant DMR 0907781. P. G.-M. was partially supported by the NSF grant DMR-05205

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Date submitted: 29 Dec 2009 Electronic form version 1.4