

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nanoparticle interactions in electrolyte solutions: A classical density functional theory and molecular dynamics study K. MICHAEL SALERNO, AMALIE L. FRISCHKNECHT, MARK STEVENS, Sandia National Laboratories — We know that multivalent ions can dramatically alter the interactions between macroions, and we are interested in the fundamentals of nanoparticle interactions. We performed molecular dynamics (MD) simulations at the primitive model level and classical fluids density functional theory (DFT) calculations of negatively charged interacting nanoparticles, 2 - 7 nm in diameter, in solution with 1:1, 1:2, or 1:3 salt. We found qualitative agreement between the MD simulations and DFT calculations for the ion density profiles around the nanoparticles and for the interaction free energy between two nanoparticles. As expected, the nanoparticle interaction free energies depend strongly on the cation valence, with pure repulsion for a 1:1 salt, changing to attraction for multivalent cations due to formation of charge ordered structures. Attractive free energy depths can reach 10 kT for 7 nm diameter nanoparticles, indicating that kinetic arrest and aggregation may occur. The interaction free energies depend non-monotonically on the nanoparticle charge due to layering of the counterions around the nanoparticles for large nanoparticle charges.

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Date submitted: 05 Nov 2015

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