Abstract Submitted
for the DFD12 Meeting of
The American Physical Society

Numerical Simulation of Nanoparticle Clustering with Experimental Validation[1] ZHIGANG FENG, GREGORY SLOAN, KIRAN BHAGANAGAR, University of Texas at San Antonio, DEBYJOTI BANERJEE, Texas A&M University — In this study a numerical approach for modeling the forces acting on nanoparticles was performed and the dynamics of transient nanoparticle agglomeration have been explored. The validity of the approach is demonstrated by examining a pair of nanoparticles in a fluid. The force interactions due to the presence of the electric double layer (EDL) were identified as a significant factor in determining the propensity for agglomerative of the nanoparticles. Simulations were performed to demonstrate the clustering and agglomeration of an ensemble of nanoparticles. The simulation results provide an estimate for the time scale for the agglomeration and the resultant structure of the agglomerated ensemble of nanoparticles. Subsequently simulations were performed using this numerical model corresponding to the available experimental data in the literature. The predictions from the numerical simulations show that the change in zeta potential (determined in part by the pH of the solvent phase) is a crucial parameter that affects the level of agglomeration of the nanoparticles.

[1]Supported by the Natioanl Science Foundation under award number HRD-1137764.

Zhigang Feng
University of Texas at San Antonio

Date submitted: 07 Aug 2012 Electronic form version 1.4