Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Optimum Atomic Ranges in Coupled Dipole Method[1] HYE-YOUNG KIM, ZACHARY BOND, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA — In recent years, the coupled dipole method (CDM) has been applied to calculate the van der Waals dispersion interaction (VDW) between dielectric nanoclusters. Similar self-consistent method has also been used to calculate the static polarizabilities, from which the fully-retarded VDW was calculated. The breakthrough in CDM is that it can calculate all n-body terms in VDW. This allows for significant improvement upon the usual 2-body description of VDW. As the size of nanocolloids increases close to the experimentally measurable size, however, solving for eigenvalues of a large matrix (with all n-body interactions) in CDM becomes non-trivial. Since each interaction term decreases as the separation distance becomes large, certain atomic ranges within which the VDW would converge is expected in large systems. Identifying this range will improve the efficiency of CDM. Here, we report the results of a systematic study on the optimized maximum atomic ranges in CDM for different shapes and sizes of clusters. REF: Langmuir 23, 1735 (2007).

[1]Work supported by the U. S. Department of Energy Basic Energy Sciences grant DOE-FG02-07ER46414 and conducted at the Center of Nanophase Materials Sciences, which is sponsored at Oak Ridge National Lab by the Division of Scientific User Facilities, DOE.

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Date submitted: 19 Nov 2007 Electronic form version 1.4