Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Van der Waals forces between nanoclusters: importance of many-body effects HYE-YOUNG KIM, JORGE SOFO, Physics Department, The Pennsylvania State University, University Park, PA, DARRELL VELEGOL, Chemical Engineering Department, The Pennsylvania State University, University Park, PA, MILTON COLE, Physics Department, The Pennsylvania State University, University Park, PA, AMAND LUCAS, Physics Department, University of Namur, Begium
— Van der Waals (VDW) interactions between nanoclusters have been calculated using a self-consistent, coupled dipole method. The method accounts for all multi-body (MB) effects and can be used to calculate dispersion interaction energies between nanoclusters of arbitrary shape. Comparison is made between the exact potential energy, V, and the values obtained with two alternative methods: $V^{(2)}$, a sum of two-body interactions, and $V^{(2)}+ V^{(3)}$, the sum of 2-body and 3-body interactions. For some clusters and orientations, $V^{(2)}$ is close to the exact result. In other situations, MB effects can be large. For all cases considered here, the 3-body term alone does *not* accurately represent the MB contributions to V. MB contributions are especially important for shape-anisotropic clusters.

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Date submitted: 21 Nov 2005 Electronic form version 1.4