

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic Coupling and Optimal Gap Size within a Metal Nanoparticle Dimer¹ KE ZHAO, CLAUDIA TROPAREVSKY, University of Tennessee and Oak Ridge National Laboratory, DI XIAO, Oak Ridge National Laboratory, ADOLFO EGUILUZ, University of Tennessee and Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory and University of Tennessee — We study the electronic coupling between two metal nanoparticles using density functional theory methods. We show that a continuous change in the particle separation leads to an abrupt transition from strong to weak electronic coupling, which defines an optimal separation for the dimer. While in the weak-coupling regime the dimer behaves like isolated clusters, its crossing into the strong-coupling regime is signified by two distinct phenomena, namely, the onset of a net magnetic moment, and a maximum in the static polarizability. We also show that as the system switches over from strong to weak coupling regime, the response to an applied electric field is nonlinear even for very small fields. The strong dependence of the coupling on the atomic structure of the nanoparticles and their orientation is also discussed. Our study is expected to have an impact on a variety of systems composed of aggregates of nanoparticles.

¹Work supported by DMSE/BES of DOE, NSF and PCSCS/CMSN programs

Ke Zhao
University of Tennessee, Oak Ridge National Laboratory

Date submitted: 20 Nov 2008

Electronic form version 1.4