Abstract Submitted
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Inter-particle coupling and polarizability of silver nanoparticle dimers[1] KE ZHAO, CLAUDIA TROPAREVSKY, University of Tennessee & Oak Ridge National Laboratory, ADOLFO EGUILUZ, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee, THEORETICAL CONDENSED MATTER PHYSICS AT UNIVERSITY OF TENNESSEE & OAK RIDGE NATIONAL LABORATORY COLLABORATION — Using a real-space implementation of density-functional theory, we investigate systematically the electronic/chemical coupling of two silver nanoparticles of varying sizes. The nanoparticles are allowed to approach each other along two distinct directions defined by, respectively, maximum and minimum static polarizabilities. We show that, as the inter-particle separation decreases, the static polarizability of the dimer shows signatures of crossover to a strong-coupling regime. Moreover, we analyze the connection between the crossover from weak to strong coupling regimes of the nanoparticles and the electron density overlap from the states contributed by the individual nanoparticles. The significance of these results will be discussed in connection with the prevailing theories of the electromagnetic enhancement of surface-enhanced Raman scattering.

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