Abstract Submitted
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Tuning the Coupling of Molecular Species with Metal Nanoparticle Dimers[1] M. CLAUDIA TROPAREVSKY, University of Tennessee, KE ZHAO, Rice University, DI XIAO, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory and University of Tennessee — Recently, we have studied the electronic coupling between metal nanoparticles using real-space first-principles calculations within density functional theory [1, 2]. Here, we investigate the effect of placing a molecule in the gap region between the nanoparticles on the linear response of the system to an applied electric field. We find that the values of the static polarizability are significantly larger than in the case where the molecule is absent. We also investigate the role of the electronic coupling between the nanoparticles on the binding energies of oxygen and carbon monoxide. We show that the binding energies change significantly when the separation between the nanoparticles is varied. Finally, we explore the effect of applying an electric field on these binding energies which may emerge as a novel way of tuning the chemical reactivity of metal nanoparticles aggregates.

[1] K. Zhao, M. C. Troparevsky, D. Xiao, A. G. Eguiluz, and Z. Zhang, Phys. Rev. Lett. **102,** 186804 (2009).
[2] M. C. Troparevsky, K. Zhao, D. Xiao, Z. Zhang, and A. G. Eguiluz, Nano Lett. (2009).

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