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Accurate tuning of the electronic coupling and emergent magnetic properties of metal nanoparticle dimers from the linear to nonlinear dielectric-response regime¹

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Closely-packed nanoparticle aggregates have sparked great interest in recent years due to their potential applications in new functional materials and devices at the nanoscale. Experimentally, it has been demonstrated that the properties of such aggregates crucially depend on the electronic coupling between nanoparticles. This coupling originates from the overlap of electronic wavefunctions between neighboring particles, thus requiring a full quantum-mechanical treatment. In this talk, I will discuss the tuning of the electronic coupling via particle separation and external electric field, as well as its effect on the dielectric and magnetic properties of a nanoparticle dimer system [1,2]. Using atomistic real-space first-principles calculation, we find that there is an optimal separation at which the static polarizability reaches its maximal value. Such a peak structure is completely missing in the classical electromagnetic theory, and is associated with the “bond”-breaking process between the two nanoparticles. In some systems, the electronic coupling can be strong enough to give rise to a net magnetic moment of the dimer, even though the isolated nanoparticles are nonmagnetic. Furthermore, we show that the electronic coupling can be tuned by a modest electric field, resulting in an electric-field tunable magnetic moment. We discuss these results in the context of spin-polarized molecular transport, nanoscale multiferroics, and nanoplasmonics. [1] K. Zhao, M. C. Tropicovsky, D. Xiao, A. G. Eguiluz, Z. Y. Zhang, Phys. Rev. Lett. 102, 186804 (2009). [2] M. C. Tropicovsky, K. Zhao, D. Xiao, Z. Y. Zhang, and A. G. Eguiluz, “Tuning the Electronic Coupling and Magnetic Moment of a Metal Nanoparticle Dimer in the Nonlinear Dielectric-Response Regime”, to be published in Nano Lett.

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