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Free energy change for aggregation of charged monolayer-protected gold nanoparticles REID VAN LEHN, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Monolayer-protected gold nanoparticles (AuNPs) are an important class of nanomaterials with applications in drug delivery and biosensing. However, the utility of AuNPs is limited by the spontaneous aggregation of particles in solution, which is observed even for highly charged, water-soluble AuNPs. Such aggregation cannot be well-described by continuum theories that would predict the dominance of repulsive electrostatic interactions over weaker van der Waals interactions. In this work, we show that small AuNPs (diameter <10 nm) protected by charged alkanethiol monolayers may aggregate due to a ligand-mediated short-range attraction that compensates for electrostatic repulsion. The short-range attraction is driven by the hydrophobic effect as the flexible ligands deform to shield hydrophobic surface area from water. We use novel simulations to calculate the free energy change for bringing two AuNPs together from infinite separation and show that the free energy change depends on particle size, monolayer composition, and the surrounding environment. This work provides insight into the key role that ligand interactions play in AuNP aggregation and suggests guidelines for the design of protecting monolayers.

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