An Investigation of Bonding in Gold Nanodot Systems

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Chemical bonds that are thought to form and break during the surfactant-mediated synthesis of gold nanodots have been studied via Density Functional theory. A relaxed potential energy surface scan has been performed for each bond using the hybrid UB3LYP functional and the dissociation energy has been further corrected using the generalized gradient PW91 correlation and exchange functionals. Dodecane thiol has been used as the surfactant and the bonds studied include Au-Au, Au-SH, HS-SH, Au-H, HS-H, and H-H. These two-bodied potentials will serve as input to an on-lattice Monte Carlo simulation and eventually to an off-lattice molecular dynamics simulation. Correlation error associated with the two-bodied potentials has been examined and has been reduced by using a configuration interaction of singles and doubles (CISD). Future work may include the effect that the shape and size of the cluster has on the gold-thiol bond energy. Also, valence bond theory can be used to further account for correlation energy.