

Abstract Submitted
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Theoretical Investigation on Cysteine Interactions with Gold Nanoparticles JESSICA CARR, HONG WANG, JAMES LEWIS, Physics Department, West Virginia University, Morgantown, WV 26506-6315 — Gold nanoparticles have been intensely investigated due to wide applications in colloidal chemistry, catalysis, medical science, etc. Lately, experiments have shown that ligand-stabilized gold nanoparticles provide a platform for precisely probing the structural and electronic properties of isolated gold nanoparticles, allowing us to further understand the interaction between gold nanoparticles and attaching ligand molecules. Using density functional theory approach, we investigate a series of gold nanoparticles with a size scale of 0.5 to 2 nm that are passivated by a monolayer of cysteine molecules [R-SH, with R=CH₂CH(COOH)(NH₂)]. There is a controversy about the attaching pattern of the cysteine monolayer around the gold nanoparticles. We speculate that there is hydrogen bonding between the cysteine molecules, leading to stabilized gold nanoparticles. This research shows potential hydrogen bonding forming with the gold nanoparticle surface, as well as hydrogen bonding between cysteine molecules.

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