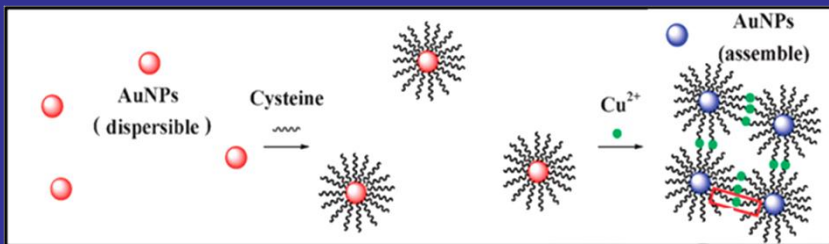
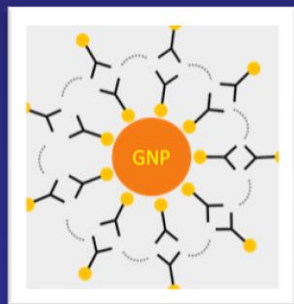
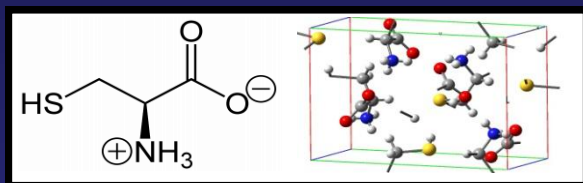


# Theoretically Exploring Electronic-Transfer Pathways of Hot Electrons in Organically-Assisted Metal Catalysts

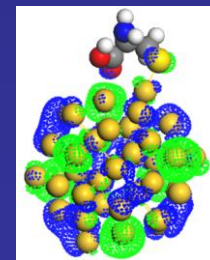
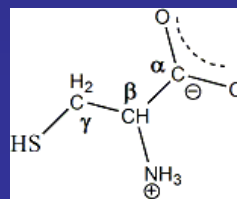


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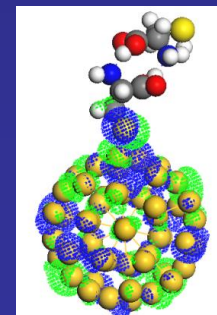
Au-based catalysts are a promising solution to energy- and environmental-related challenges. Unlike bulk phase, nanosized Au particles are unstable and thereby present significant catalytic activity for several valuable reactions, such as oxidation of alcohol, homocoupling of arylboronic acids, etc. We choose to theoretically investigate Au nanoparticles stabilized by organic-ligands as a simplified model system to understand the fundamental properties and underlying mechanisms of organically-assisted Au-based catalysis.



In this study, we investigated two possible attaching modes of L-cysteine molecules on the gold nanoparticle, Au<sub>55</sub>. We found that cysteine bonds strongly to the gold nanoparticle via a strong Au-S interaction. Furthermore, cysteine can arrange in either a monolayer or bilayer configuration around the nanoparticle, which determines whether or not it has a zwitterion structure. In the bilayer model, the cysteine zwitterion structure is stabilized via the H-bonding between inner layer cysteine and outer layer cysteine. With the outer layer as a charge balance shell, the inner layer cysteine tends to anchor to gold particle via stronger interaction. The three type carbon atoms (C<sub>α</sub>, C<sub>β</sub> and C<sub>γ</sub>) of inner layer and outer layer present the similar trend in terms of charge changes as what observed in solid NMR spectrum. Overall, we propose the bilayer model is a possible arranging format for cysteine anchoring to gold nanoparticles, which enables the outer layer sulfur atoms to serve as open portal for further bio-functional modification.



monolayer



bilayer