Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form - DTU Orbit (08/11/2017)

Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form

The synthetic chemistry and spectroscopy of sulfur-protected gold surfaces and nanoparticles is analyzed, indicating that the electronic structure of the interface is Au(0)-thiyl, with Au(I)-thiolates identified as high-energy excited surface states. Density-functional theory indicates that it is the noble character of gold and nanoparticle surfaces that destabilizes Au(I)-thiolates. Bonding results from large van der Waals forces, influenced by covalent bonding induced through *s-d* hybridization and charge polarization effects that perturbatively mix in some Au(I)-thiolate character. A simple method for quantifying these contributions is presented, revealing that a driving force for nanoparticle growth is nobleization, minimizing Au(I)-thiolate involvement. Predictions that Brust-Schiffrin reactions involve thiolate anion intermediates are verified spectroscopically, establishing a key feature needed to understand nanoparticle growth. Mixing of preprepared Au(I) and thiolate reactants always produces Au(I)-thiolate thin films or compounds rather than monolayers. Smooth links to O, Se, Te, C, and N linker chemistry are established.

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