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Ab initio DFT study of the adsorption of thiol molecules on Au nanoparticles[1] HECTOR BARRON, LUCAS FERNANDEZ-SEIVANE, UTSA, MONICA OLVERA DE LA CRUZ, Northwestern University, MIGUEL JOSE-YACAMAN, XOCHITL LOPEZ-LOZANO, UTSA, UTSA-NW COLLABORATION — Recent studies have shown that the Au nanoparticle surface has a strong binding affinity towards thiols, in which the thiol–Au interface allows the surface conjugation of various peptides, proteins, and DNA. Notwithstanding the interaction between Au–Au and thiol–Au are still under debate mainly because of the difficulty to consider a sufficient number of Au-molecule configurations, the large-scale atomistic simulations have been based on old ab initio DFT data, while the process of adsorption have not been completely understood or properly taken into account. In this work the adsorption of methyl-thiol molecules on Au55 gold clusters is investigated by performing density functional theory (DFT) calculations within the generalized gradient approximation (GGA) with the SIESTA code. Different conformations of methyl-thiol-Au55 systems were treated founding that the methyl-thiol molecule prefers to be adsorbed on the Top and Bridge sites, which are energetically more favorable for the adsorption. These results will provide valuable information regarding the fundamental interactions and behavior of methyl-thiol passivated Au nanoparticles.

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