

Abstract Submitted
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Systematic Study of the Adsorption of Thiol Molecules on Noble-Metal Nanoparticles¹ H. BARRON, University of Texas at San Antonio, F. HIDALGO, Universidad Nacional Autonoma de Mexico, L. FERNANDEZ-SEIVANE, University of Texas at San Antonio, C. NOGUEZ, Universidad Nacional Autonoma de Mexico, X. LOPEZ-LOZANO, University of Texas at San Antonio — The study of the interaction between nanoparticles and different types of ligands has been intensively investigated in the last years due to the potential contribution of their properties to the nanotechnology device design. These properties have opened new research fields like plasmonics, with interesting applications in optics, electronics, biophysics, medicine, pharmacology and materials science. Self-assembly monolayers have been thoroughly studied at experimental and theoretical level on extended (111) gold and silver surfaces. However, nanoparticle and molecule properties after the adsorption are still not well understood due to the different factors involved in this process such as the adsorption sites, size and element type of the nanoparticle. In this work we have performed a systematic study of the adsorption of methyl-thiol molecules on Au₅₅ and Ag₅₅ clusters through density functional theory calculations with the SIESTA code. Different adsorption modes of the methyl-thiol molecule on Au₅₅ and Ag₅₅ were considered. In general, for both type of nanoparticles, the methyl-thiol molecule prefers to be adsorbed on the Bridge sites. These results provide valuable information of the structural and electronic properties of methyl-thiol passivated Au and Ag nanoparticles.

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