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Enantiospecific adsorption study at chiral gold nanoclusters from DFT calculations[1] XOCHITL LOPEZ-LOZANO, Instituto de Fisica, UNAM, Mexico., LUIS A. PEREZ, IGNACIO L. GARZON — Chiral structures have been found as the lowest energy isomers of bare and passivated gold nanclusters from density functional theory (DFT) studies. Recently, experimental evidence on the existence of chiral gold nanoclusters has been published. In this work, DFT calculations are performed to study the adsorption of chiral molecules (like cysteine) on chiral and achiral (icosahedral) Au_{55} clusters. Different locations on the metal cluster surfaces are used to identify the most favorable adsorption sites of the chiral molecule. Enantioselectivity is investigated through the comparison of the binding energies of the (S) and (R)-cysteine molecule adsorbed on the different Au_{55} cluster enantiomers.

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