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Enantiospecific adsorption of chiral molecules on chiral Au clusters IGNACIO L. GARZON, XOCHITL LOPEZ-LOZANO, LUIS A. PEREZ, Universidad Nacional Autonoma de Mexico — Enantioselectivity in gold clusters is investigated by studying the adsorption of a chiral amino acid (cysteine) on a chiral Au₅₅ cluster using density functional calculations. The highest adsorption energies were found when the amino and thiolate functional groups of cysteine are bonded to the lowest coordinated edges of the chiral cluster. Enantiospecific adsorption is primarily obtained from the different bond location and strength, at the cluster edge, of the carboxyl groups forming the left- and right-handed enantiomers. These results provide theoretical support to convey enantioselectivity in asymmetric nanocatalysts using chiral gold clusters.

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