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Structural and electronic properties of chiral gold nanoclusters
IGNACIO GARZON, ITZEL SANTIZO, LUIS PEREZ, Universidad Nacional Autonoma de Mexico — Chiral structures had been found as the most stable isomers of bare and thiolate-passivated gold nanoparticles of several sizes, from density functional calculations (DFT). These results provided theoretical support for the existence of chirality in metal clusters, suggested by the intense optical activity measured from the metal-based electronic transitions of size-separated glutathione-passivated gold nanoclusters, and more recently, of penicillamine-passivated gold clusters with metal core mean diameters of 0.57, 1.1, and 1.75 nm. A further structural analysis using the Hausdorff chirality measure, as well as, a semiclassical calculation of the circular dichroism spectrum, has confirmed the existence of chirality in Au nanoparticles. In this work, the structural and electronic properties of chiral Au nanoclusters are studied by using global optimization methods combined with semiempirical many body potentials and first principles density functional calculations. In particular, we study the Au_{34} cluster. For this system there exists experimental evidence on the energetic stability of a chiral structure with C_3 symmetry. Our calculations theoretically confirm these results, providing further evidence on the existence of chiral gold nanoclusters.

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