

Abstract Submitted  
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**Chirality in Metallic Clusters** IGNACIO L. GARZON, LUIS A. PEREZ, Universidad Nacional Autonoma de Mexico — In this work, we present a theoretical study on the structural, vibrational, electronic, and optical properties of chiral bare gold clusters. We consider the case of the  $\text{Au}_{34}^-$  cluster for which extensive experimental studies on its structural and electronic behavior had been published recently. Our results show that the lowest-energy isomers of the  $\text{Au}_{34}^-$  cluster correspond to two chiral structures with  $C_1$  and  $C_3$  point symmetry groups, being the  $C_1$  isomer slightly more stable than the  $C_3$  one. The calculated structure factors, which have been measured using trapped ion electron diffraction, indicate that these isomers are almost indistinguishable. On the other hand, their electronic DOS show different features around the HOMO-LUMO energy gap, which may be detected through optical spectroscopies. In fact, our calculated absorption and circular dichroism spectra show clear differences in the optical behavior of these chiral clusters. Another important property that distinguishes the  $C_1$  and  $C_3$  isomers is the different spatial distribution of the atomic coordination on the cluster surface, which would generate distinct enantiospecific adsorption patterns with chiral molecules. These results confirm the existence of intrinsically chiral bare gold clusters.

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