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Rich Information on Quantum States and Ways to Calculate It in The Absorption Spectra of Au_{144} Gold Cluster Compound XOCHITL LOPEZ-LOZANO, ROBERT L. WHETTEN, Department of Physics & Astronomy, The University of Texas at San Antonio, HANS-CHRISTIAN WEISSKER, Aix-Marseille Univ., CNRS, CINaM — In recent decades, the prevalent view has been that noble-metal clusters of intermediate size necessarily have smooth optical absorption spectra of low information content in the near-IR, VIS and near-UV regions. At most, one expects a broad, smooth localized surface plasmon resonance feature. Recently, we demonstrate that, in contradistinction to the commonly held view, the optical absorption of the most widely applied gold cluster, the thiolate-protected Au_{144} cluster, exhibits a rich spectrum of bands that are individually visible over the entire near-IR, VIS and near-UV regions (1.0-4.0 eV), demonstrating high information content related to the quantum size effects which distinguish the nanoparticles from the bulk materials. In the calculation, the result is sensitive to the details of the structure. In the present work, we systematically compare the different structures actually used to date. We studied aspects like symmetry, geometry and type of ligands. In particular, we discuss the effect of their differences on the optical absorption spectra as well as how the theoretical methodology influences the final results.

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