A superatomic molecule under the spin-orbit coupling: Insights from the electronic properties in the thiolate-protected Au38(SR)24 cluster

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The role of the spin-orbit coupling in Au38(SR)24, as a representative case for a superatomic molecules is studied to offer a complete view of the relativistic effect in heavy elements clusters. Its Au23 9+ core can be described in as an analog to a diatomic molecule, such as F2, allowing the electronic structure to be depicted in terms of the D?h point group. First, we showed the electronic structure under the spin-orbit framework using total angular momentum representations (j = ? ± s; spinors), which allows us to characterize the expected splitting of certain levels derived from the cluster core. Accordingly, the optical properties are evaluated under spin-orbit coupling regime, revealing differences in the low-energy region of the absorption spectrum. Lastly, the variation of electron affinity (EA) and ionization potential (IP) properties is evaluated. This reveals characteristic consequences of the inclusion of spin-orbit coupling in Au38(SR)24, as a bridge to larger thiolate-protected gold clusters. © 2017 Wiley Periodicals, Inc.

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