

Abstract Submitted  
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**Composition Dependence of the Properties of Noble-metal Nanoalloys**<sup>1</sup> LUCAS FERNÁNDEZ SEIVANE, HÉCTOR BARRÓN, JAMES BENSON, University of Texas at San Antonio, HANS-CHRISTIAN WEISSKER, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM-CNRS), XOCHITL LÓPEZ-LOZANO, University of Texas at San Antonio — Bimetallic nanostructured materials are of greater interest both from the scientific and technological points of view due to their potential to improve the catalytic properties of novel materials. Their applicability as well as the performance depends critically on their size, shape and composition, either as alloy or core-shell. In this work, the structural, electronic, magnetic and optical properties of bimetallic Au-Ag nanoclusters have been investigated through density-functional-theory-based calculations with the Siesta and Octopus codes. Different symmetries -tetrahedral, bipyramidal, decahedral and icosahedral- of bimetallic nanoparticles of 4-, 5-, 7- and 13-atoms, were taken into account including all the possibly different Au:Ag ratio concentrations. In combination with a statistical analysis of the performed calculations and the concepts of the Enthalpy of Mixing and Energy Excess, we have been able to predict the most probable gap and magnetic moment for all the composition stoichiometries. This approach allows us to understand the energy differences due to cluster shape effects, the stoichiometry and segregation. In addition, we can also obtain the bulk energy and surface energy of Au-Ag nanoalloys by looking at fixed number of atoms and fixed morphologies.

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Lucas Fernandez Seivane  
University of Texas at San Antonio

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