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First principles studies of the geometric and electronic structure of nanoalloy $Ag_{27}Cu_7$.[1] M. ALCANTARA ORTIGOZA, Kansas State University, T.S. RAHMAN, University of Central Florida — We present first-principles calculations of the structure and electronic density of states (DOS) for the perfect core-shell $Ag_{27}Cu_7$ nanocluster. Our results show an expansion of 0.4 A in the *diameter* of the cluster compared with previous results*. From the projected DOS we conclude that the 34-atom cluster has only 2 non-equivalent Cu atoms (core) and 4 non-equivalent Ag atoms (shell), confirming that this finite-size structure has D_5h symmetry. The HOMO-LUMO gap is found to be 0.77 eV, in agreement with previous results*. Comparing with Ag bulk, the valence band centroid of $Ag_{27}Cu_7$ presents shift of ∼1.0 eV towards the Fermi energy, but a 0.5 eV shift away from it, compared with Cu bulk. The total DOS of the structure as a whole does not present valence band narrowing when compared to the bulk of either species. Individual Ag atoms show band narrowing, a positive centroid shift to lower binding energies, and a very small enhancement of the DOS at the top of the band. Electronic states of Cu atoms are greatly concentrated in two sharp peaks in the top region of their valence band. In the bottom of the band, however, copper and silver atoms hybridize in spite of their short d-wavefunctions. Charge density plots give some insight about the hybridization of electronic states between atoms. *G. Rossi et al. Phys. Rev. Lett. **93,** 105503 (2004).

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