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Tailoring the Electronic Structure by Alloying: $\mathbf{Ag_nCu_{34-n}}$ Nanoparticle Family[1] HANDAN YILDIRIM, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — We report results of first principles calculations of the electronic structure of the Ag_nCu_{34-n}bi-metallic nanoparticle family where n=0, 1, ..., 34. We find that alloying of the pure Ag cluster with a few Cu atoms displays substantial changes in the electronic structure but the reverse is not the case when few Ag atoms are substituted in pure Cu clusters. We find that local environment control the length and the strength of the Cu-Ag bonds. The Cu atoms, which form the core display shortened bond length and present above 1 eV shift in their d-band center. The HOMO-LUMO gap for the set of nanoalloys falls in three regions: 0.19 eV to 0.31 eV, 0.40 eV to 0.57 eV, and 0.73 eV to 0.88 eV. For several nanoparticles slight change in composition may thus lead to a change of about 600 meV in the gap. The highest gap is found for the most symmetric nanoparticle ($Ag_{17}Cu_{17}$), while the lowest is for $Ag_{29}Cu_5$. We present a systematic analysis of the changes in Cu-Ag, Ag-Ag and Cu-Cu bond lengths and hybridization with composition to understand their effect on the HOMO-LUMO gap and other characteristics of the nanoparticles.

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