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Trends in the Electronic Structure and Vibrational Dynamics of 34 atom Ag-Cu Nanoalloy ($\mathbf{Ag}_n$-$\mathbf{Cu}_{34-n}$)[1] H. YILDIRIM, A. KARA, T.S. RAHMAN, Department of Physics, University of Central Florida — We report results of a systematic study of the electronic and geometric structures as well as vibrational and thermodynamical properties of Ag_nCu_{34-n}, using density functional theory and model interaction potentials. A detailed analysis of the effect of coordination and atomic environment shows the limitation of coordination to *solely* explain the changes in the structural and vibrational characteristics. On the other hand, a combination of coordination and environment, as expressed in the elemental characteristics of the neighbors, shows systematic trends in the bond length and vibrational free energy distribution. In addition, Cu atoms in the Cu-core/Ag-shell structure, with coordination 6 show a bi-modal feature with 2 distinct ranges of bond lengths. A global analysis shows that the fluctuations in the vibrational free energy depend on the elemental environment which is more pronounced in the case of copper atoms. Correlations between the d band characteristics with coordination/bond length and environment will also be discussed.

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