Structural and electronic properties of bimetallic Au_nAg_m, (n + m = 20, n:m = 1:0, 3:1, 1:1, 0:1) clusters and their ions: a relativistic DFT study

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Abstract

In recent years, the study of the Au-Ag bimetallic nanoparticles has attracted considerable attention due to the possibility of tuning their optical and electronic properties as a function of the gold and silver proportions. In general, from a theoretical point of view, the search for the lowest energy bimetallic structures presents a challenging problem due to the large number of skeletal geometric structures and homotopic distributions to be considered. Furthermore, the analysis of the Au-Ag system introduces the additional component of the relativistic effects, present in the gold atom, that have to be considered. In this work, using the relativistic approach ZORA-DFT, we report the local minima in the potential energy surface of bimetallic Au_nAg_m, (n + m = 20) clusters and their ions in selected proportions (n:m=1:0, 3:1, 1:1, 0:1) in the gas-phase. We also discussed their respective electronic properties and possible aggregation or segregation structural motifs.

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