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Trends in the structure of neutral, cationic, and anionic Ag and Au clusters from DFT calculations[1] IGNACIO L. GARZON, Instituto de Fisica, UNAM, LUIS A. PEREZ, KARO MICHAELIAN — The physical and chemical properties of small coinage metal clusters, with atomic structures $nd^{10}(n+1)s^1$ (n= 3,4,5 for Cu, Ag and Au, respectively), are of great interest since, for example, can be viewed as a bridge between those existing in the "simple" s-only alkali metal and the more complicated transition metal clusters. Several theoretical calculations and indirect experimental evidence have shown that Au_N clusters prefer planar structures up to sizes around N=13, cage-like structures for the T_d Au_{20} and I_h Au_{32} and low- symmetry (amorphous) configurations for Au_{55}. In this work, we present a theoretical study of the structural and electronic properties of Ag and Au neutral, cationic and anionic clusters with up to N =55 atoms, using density functional theory in the generalized gradient approximation. A different behavior is found in the physical properties of Ag and Au clusters, mainly due to the stronger relativistic effects present in the Au clusters. Another trend indicates that not only the size (number of atoms) and shape (isomer geometry) of a given cluster determine its properties, but also the charge present in the system may affect the cluster behavior even in the larger sizes with N=55. A discussion of the structural motifs existing in neutral, cationic and anionic Ag and Au clusters with up to N=55 atoms and their connection with recent experimental data will be presented.

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