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Atomic and Electronic Structure of Ag_n (n $\leq$ 13) Clusters and their Reactivity with O_2[1] GABRIEL U. GAMBOA, ARTHUR C. REBER, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University. — First principles theoretical studies on the atomic structure, stability, and electronic structure of neutral and anionic Ag_n clusters have been carried out within a gradient corrected density functional approach. It is shown that the clusters are marked by planar or layered structures. For most clusters, the ground state of anions has lowest spin multiplicity. To examine the reactivity of clusters, containing even number of electrons, with O_2, we calculated the spin excitation energy representing the energy required to excite the cluster to the triplet configuration. It is shown that several of these even electron anionic species and in particular Ag_{13}^- have high spin excitation energy indicating that they should be inert towards reactivity with oxygen. The theoretical predictions are shown to be in agreement with preliminary experimental data on the reactivity of anionic species.

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