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Ab initio molecular electrostatic potential of hexanuclear Cu, Ag, and Au clusters[1] ALVARO POSADA-AMARILLAS, Dept de Investigacion en Fisica, Universidad de Sonora — DFT calculations of electrostatic potential (ESP) are carried out under the PBE/SDD theory level. Planar initial structures are given as input to perform DFT optimization with the aim of obtaining ground state structures. ESP is thus calculated and results show the existence of both, nucleophilic and electrophilic sites. In each case, the latter are located over the cluster planes while the former are observed in cluster vertices. Binding energy is provided, as well as structural parameters of ground state structures.

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