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**Insights into reactivity properties of the ground state structures of  $(\text{CuS})_x$  ( $x=1-7$ ) using DFT** JONATHAN LUQUE CEBALLOS, ALVARO POSADA AMARILLAS, Dpto. de Investigacin en Fsica, Univesidad de Sonora, Hermosillo, Sonora — The extraordinary properties of nanoscale materials have generated an enormous interest in the study of nanomaterials, because of the difference of their properties as compared to the corresponding bulk materials. Polyatomic nanomaterials have become important in recent years, due to the possibility of synthesize new materials with similar or better physical and chemical properties, than those of the monoatomic materials, or with a lower cost, to be used in technological applications in medicine, biology, electronics, or catalysis. Among these materials, copper sulfide is one of the transition metal chalcogenides that exhibits different stoichiometric forms with crystal structure varying from orthogonal to hexagonal. In this work we obtained the ground state structures of cooper sulfide nanoparticles  $(\text{CuS})_x$ ,  $x=1-7$ . The corresponding frontier orbitals (HOMO and LUMO) are analyzed, and different reactivity parameters are obtained. We also present the molecular electrostatic potential, which is used to determine the higher and lower electron density regions on the clusters' structure. All calculations were performed using the TZVP basis set for S and the Christianssen-Ermler pseudopotential for Cu, employing two different exchange-correlation functionals, PBE and PBE0.

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