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Theoretical Analysis of Copper Sulfide Nanoalloy Clusters: A Density Functional Study

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Abstract—*Bimetallic nanoclusters are widely used as heterogeneous catalysts due to their structural diversity along with their high surface/volume ratio. Recently, possible utilization of heterogeneous nanomaterials as semiconductor electrodes in Photo Electrochemical Cells (PEC) has been reported. Copper sulfides (CuS) have gained a huge attention due to its high adsorption property and non-toxic behaviour. In this analysis, nanoalloy clusters of $(CuS)_n$; (n=1-8) have been systematically investigated invoking Conceptual Density Functional Theory (CDFT) based descriptors, aiming to provide deep insights about its electronic and other properties. Global DFT based descriptors have been computed for ground state configurations of $(CuS)_n$ nanoalloy clusters. Our computed HOMO-LUMO gaps which are in the range of 1.25 – 3.53 eV, indicate about efficacy of (CuS)n clusters in terms of renewable energy sources specially in photocatalysis and solar cell applications. A nice correlation has been established between electronic and photo catalytic properties of copper-sulfide clusters and their computational counterparts. The close agreement between experimental bond length and our computed data supports our analytical approach.*

Keywords*: Density Functional Theory; HOMO-LUMO Gap; hardness; electrophilicity index.*