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Theoretical Study of Cage Clusters of $Zn_{48}O_{48}$, $Zn_{48}S_{48}$ and $Zn_{48}Se_{48}$

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Abstract: *In this study, we have modulated $Zn_{48}X_{48}$ clusters (where X= O, S, Se) using density functional theory. Initially structural, electric, magnetic and optical properties have been investigated. The study compared with earlier work. We tried to investigate, whether these clusters are suitable as shell material to cover any magnetic iron-oxide material. To study core material which do not affect magnetic property of host material we have chosen ZnO material as a shell material along with ZnS and ZnSe materials. In this study we found that all three cage structures are suitable structures with Th symmetry. Cage clusters are found diameter in the range of 12.15 Å to 14.76 Å. These clusters are found to be nonmagnetic in nature. Optical properties of these clusters show transparency in visible and ultraviolet region. Hence such cage clusters are suitable to hold magnetic materials inside it so as to form a core-shell clusters..*

Keywords: Cage Clusters, nonmagnetic, core-shell clusters.

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