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Study of the structural and spectroscopic properties of Zn based clusters by density functional theory VENKATA CHAGANTI, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — ZnS, ZnSe, and ZnTe in the solid phase are semiconductors and have been extensively studied for their possible applications in semiconducting industry. The small clusters (aggregates of atoms containing a few tens of atoms) of semiconductors and metals often adopt very different shapes than the fragments of these materials in the bulk phase. The present work is devoted to understanding the structural and electronic properties of small clusters of the zinc based semiconductors with particular focus on the clusters of ZnS. The equilibrium structures of clusters are obtained by local optimization (conjugate gradient) by starting with several possible atomic configurations. The calculations are performed using advanced electronic structure package called NRL-MOL. This package uses density functional theory. The calculations are free from pesudopotential approximation i.e. both valences as well as core electrons are explicitly treated in calculations. The nature of each local minimum (structure) is analyzed by computing the vibrational frequencies within the harmonic approximation. The electronic properties such as ionization energies, the band gap (HOMO-LUMO gap), and electron affinity are obtained for all stable structures. Additionally, spectroscopic properties such as infra-red and Raman spectra are obtained which will be helpful in possible detection and identification of these clusters in experiment. The evolutions of all these properties are studied as a function of the size of clusters.

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