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Intermediate size ZnS cages : energetics and stability JOSE RODRIGUEZ LOPEZ, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We have studied intermediate size $(ZnS)_n$ cages (n=12, 16,24,36,48, and 96) using density functional theory. Such cage structures have been observed previously in classical molecular dynamics simulations. Our DFT calculations show they these structures are energetically stable. We have further calculated the vibrational frequencies of these cages. Our vibrational analysis show that these cages are local minima on the potential energy surface. The (ZnS)96 has a onion-like structure. We have also calculated the molecular electrostatic charges on the Zn and S atoms to study the ground state charge transfer to determine the ionicity of the ZnS bonds. The quasiparticle and the lowest singlet gaps are obtained using the delta-SCF and time dependent density functional theory.

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