First-principle Study of Electronic Properties of Zincblende and Rocksalt Structures of ZnS

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Semiconductor materials are very important for application in the fields of optical device technology. ZnS is wide-gap semiconductor that is attractive material due to the polymorphic structural transformation. Moreover, it has many applications in infrared optics, ultraviolet laser devices, electronic image display, high-density optical memory, solar cell etc. We present ab-initio calculations of structural parameters and electronic properties of ZnS in the structures of B1(rocksalt) and B3(zincblende) at 0 GPa. pressure and also at the phase transition pressure from the B3 to the B1 structures. The calculations are based on density functional theory (DFT) within the generalized gradient approximation (GGA) for the exchange-correlation potential. We report that the electronic properties of ZnS under phase transition pressure are quite different from those under ambient pressure. The calculated results are consistent with the experimental and other theoretical calculations.