Theoretical Study of the Structural and Electronic Properties of the Tetragonal Chalcopyrite Compound $ZnTiS_2$

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This investigating study of the tetragonal chalcopyrite $ZnTiS_2$ compound ($Zn_{0.50}Ti_{0.50}S$ alloy) is focused on its structural and electronic properties, where it is established on the first-principles linearized augmented plane wave with local orbitals (FP-LAPW + LO) method within the spin-polarized density functional theory (spin-DFT). The exchange–correlation energy was defined by the generalized gradient approximation (GGA) for the calculating of the structural parameters, whereas both GGA and GGA + U approximations are applied to compare the electronic properties of this compound (U is the Coulomb repulsion energy). The structural prediction demonstrates that the stable state of this compound is the ferromagnetic phase, where the equilibrium lattice constant a_0, bulk modulus B_0, and its first pressure derivative B' are all computed in all paramagnetic, ferromagnetic, and anti-ferromagnetic phases. The electronic study unveils the perfect half-metallic behavior within the tetragonal chalcopyrite $ZnTiS_2$ system.

Keywords: tetragonal chalcopyrite $ZnTiS_2$ compound, structural properties, electronic properties, FP-LAPW + LO, GGA + U.

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