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Pressure effect on mechanical stability and optoelectronic behavior of Zinc-Silicon Diarsenide ZnSiAs_2 -Chalcopyrite: DFT investigation.

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Abstract

The effect of hydrostatic pressure on the mechanical stability and optoelectronic behavior of zinc silicon diarsenide (ZnSiAs_2) chalcopyrite were investigated by FP-(L)APW+lo method in the framework of the density functional theory (DFT). The exchange-correlation functional GGA-PBEsol was used for the prediction of structural and electronic properties. It was used also with the modified Becke-Johnson potential "TB-mBJ" for the prediction of the optoelectronic properties of ZnSiAs_2 . The values of the structural parameters, in particular lattice parameters, bulk modulus and its pressure derivative are close to the found values. The study of mechanical stability by the elastic model through generalized stability criteria confirms that ZnSiAs_2 is stable mechanically under a pressure less than 10 GPa. The elastic anisotropy of Young's modulus along (100), (110) and (111) planes was also studied. Band-gap calculated by TB-mBJ is very close to the experimental found values, which highlights the success of the TB-mBJ potential in the prediction of electronic properties. The calculation of the refractive index as well as the birefringence of the ZnSiAs_2 by the use of GGA-PBEsol and TB-mBJ resulted in values close to those found experimentally and theoretically.

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Keywords: ZnSiAs_2 ; FP-(L)APW+lo; mechanical stability; Young's modulus; Optoelectronic

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