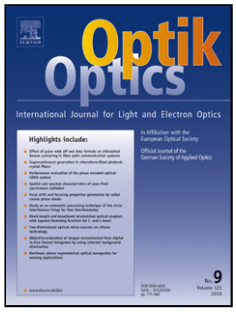

Title: Pressure effect on mechanical stability and optoelectronic behavior of Zinc-Silicon Diarsenide $ZnSiAs_2$-Chalcopyrite: DFT investigation

Authors: D. Kerroum, H. Bouafia, B. Sahli, S. Hiadsi, B. Abidri, A. Bouaza, M.A. Timaoui

PII: S0030-4026(17)30395-9
DOI: http://dx.doi.org/doi:10.1016/j.ijleo.2017.04.005
Reference: IJLEO 59047

To appear in:

Received date: 3-1-2017
Accepted date: 3-4-2017

Please cite this article as: D.Kerroum, H.Bouafia, B.Sahli, S.Hiadsi, B.Abidri, A.Bouaza, M.A.Timaoui, Pressure effect on mechanical stability and optoelectronic behavior of Zinc-Silicon Diarsenide ZnSiAs2-Chalcopyrite: DFT investigation, Optik - International Journal for Light and Electron Opticshttp://dx.doi.org/10.1016/j.ijleo.2017.04.005

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

D. Kerroum[2], H. Bouafia[1,4,*], B. Sahli[1], S. Hiadsi[2], B. Abidri[3], A. Bouaza[1], M.A. Timaoui[2].
1-Laboratoire de Génie Physique, Université Ibn Khaldoun, Tiaret 14000, Algerie.
2-Laboratoire de Microscope Electronique et Sciences des Matériaux, Université des Sciences et de la Technologie Mohamed Boudiaf, département de génie physique, BP1505 El m'naouar, Oran, Algérie.
3-Laboratoire des Matériaux Magnétiques, Université Djillali Liabés, Sidi Bel-Abbes 22000, Algérie.
4-Département des Sciences et de la Technologie, Faculté des Sciences Appliquées, Université Ibn Khaldoun, Tiaret 14000, Algerie.

**** Corresponding Author:*** *hamza.tssm@gmail.com (Dr. BOUAFIA Hamza),* ***Tel: +213778149030***

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.

<InlineShape1>

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