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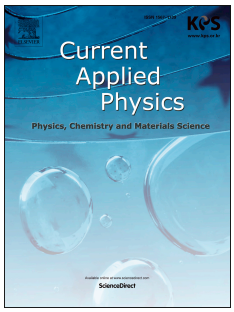


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Shahzad Yaseen, G. Murtaza, Rana M. Arif Khalil

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# Ab-initio study of Li based chalcopyrite compounds $LiGaX_2$ (X= S, Se, Te) in tetragonal symmetry: A class of future materials for optoelectronic applications

Shahzad Yaseen[a*], G. Murtaza[a**], Rana M. Arif Khalil[b]

[a]Center of advanced studies in Physics (CASP), GC University, Lahore-54000
[b]Department of Physics, Bahauddin Zakariya University, 60800, Mulatan, Pakistan
* Corresponding Author email: gmrai@gcu.edu.pk ; Tel (0923214263536)

## Abstract

Structural, electronic, optical, and thermoelectric aspects of chalcopyrite $LiGaX_2$ (X=S, Se and Te) compounds have been investigated by density functional theory (DFT) based Wien2k simulator. The optimized ground state parameters are calculated by Wu-Cohen generalized gradient approximation (WC-GGA) and electronic structures, which have been further improved by modified Becke-Johnson (mBJ) potential. Moreover, a comparative study is given among the contribution of three anions (S, Se and Te) in the same symmetry of tetragonal phase. The calculated band gaps of the studied compounds are 3.39, 2.83, and 1.96 eV for $LiGaS_2$, $LiGaSe_2$ and $LiGaTe_2$, respectively. The observed band gaps consider the studied compounds are potential materials for optoelectronic devices. In addition, the optical response of the studied materials has been analyzed in terms of dielectric constants, refraction, absorption, reflectivity and energy loss function. We have also reported the thermoelectric properties like Seebeck coefficient, thermal and electrical conductivities, and figure of merit as function of temperatures by using BoltzTrap code. The high thermal efficiency and absorption spectra in the visible region make the studied materials multifunctional for energy applications.

## Keywords

Density Functional theory; Tetragonal Phase; Li containing chalcopyrites; Direct band gap semiconductors; Optical properties; Thermoelectric investigations.