Ab initio studies of structural, electronic, optical, elastic and thermal properties of $CuGaTe_2$

© *Pravesh Singh*[1,3], *Sheetal Sharma*[1], *Sarita Kumari*[2], *Vibhav K Saraswat*[1], *D. Sharma*[4], *A.S. Verma*[1,¶]

[1] Department of Physics, Banasthali Vidyapith,
Rajasthan, 304022 India
[2]Department of Physics, University of Rajasthan,
Jaipur, 302004 India
[3] Department of Electronics and communication, K.I.E.T. Ghaziabad,
U.P. 201206 India
[4] Department of Physics, IIMT College of Engineering, Grater Noida,
U.P. 201308 India

¶ E-mail: ajay_phy@rediffmail.com

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We have performed *ab initio* calculations for the structural, electronic, optical, elastic and thermal properties of $CuGaTe_2$. In this study, we used an accurate full potential linearized augmented plane wave (FP-LAPW) method to find the equilibrium structural parameters and to compute the full elastic tensors. We report electronic and optical properties with the recently developed density functional of Tran and Blaha. Furthermore, optical features such as dielectric functions, refractive indices, extinction coefficient, optical reflectivity, absorption coefficients, optical conductivities, were calculated for photon energies up to 30 eV. The thermodynamical properties such as Debye temperature, entropy and Gruneisen parameter, bulk modulus and hardness were calculated employing the quasi-harmonic Debye model at different temperatures ($0-1000$ K) and pressures ($0-8$ GPa) and the silent results were interpreted. Most of the investigated parameters are reported for the first time.

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