

Etude des propriétés structurales , élastiques et électronique de CuS et CuTe par la méthode FP-LMTO

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Abstract : The aim of this work is to study the structural ,electronic and elastic properties of CuS. for this, we use the full-potential linear muffin-tin orbital (FP-LMTO) method in the framework of density-functional theory (DFT). The exchange and correlation energy is described in the generalized gradient approximation (GGA) using Perdew-Wang parameterization. We have investigated the effect of composition on structural properties such as lattice constants, bulk modulus and band gap. We report the results concerning the variation of the gaps and crossover of the direct, indirect band gap and bowing .Finally, a reasonable agreement is found from the comparison of our results with other theoretical calculations.

Keywords : CuS, FP-LMTO, electronic properties, elastic properties