The First-Principles Calculations On The CuI Compound

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Abstract. The ab initio total energy calculations, based on norm-conserving pseudopotentials and density functional theory, have been performed to investigate some structual, elastic, electronic and lattice dynamical properties of CuI in zinc blende (B_3) and rock-salt (B_1) structures. The calculated structural parameters, elastic moduli, band structures and the phonon dispersion curves are compared with the available experimental and the other theoretical works, and generally good results obtained. We have, also, presented the pressure dependent behaviours of the elastic constants for the same compound.

Keywords: CuI, Elastic constants, band structure, ab initio calculations, phonon diapersion curves
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CuI is the most ionic crystal with a zinc-blende structure and it shows a rocksalt structure at pressures in the region of 10 GPa. It, also, undergoes a number of structural phase transitions under pressure before attaining the rocksalt structure. The ab initio calculations, as well as others, have been extensively used to carry out its structural, elastic, electronic and lattice dynamical properties for its various phases .

An accurate and comparative description of the structural, mechanical, vibrational and electronic properties for this compound are extremely important in technological applications. In this work we, especially, focus our attention to the elastic, electronic and vibrational properties of CuI . We also present our other results at high pressures for CuI in B_1 and B_3 phases for providing some additional informations to the exisiting data.

In this work, the first-principles calculations, based on the density functional theory within the local density approximation (LDA) parametrized by Ceperley and Alder for the electronic exchange and correlation potential, and the norm-conserving pseudopotentials of Troullier–Martins, have performed using the SIESTA package (The **S**panish **I**nitiative for **E**lectronic **S**imulations with **T**housand of **A**tom). The pseudopotentials are generated for the following electronic configurations for Copper and Iodine : Cu: $4s^1 3d^{10}$,I: $5s^2 5p^5$. Well-converged results are obtained for lattice constant of CuI with the mesh-cut off energy of 100 Ryd. The core radii are taken as 2.10 Å for Cu, 2.85 Å for I. The calculated equilibrium lattice parameter (6.07 Å for B_3 structure, and 4.36 Å for B_1 structure), the bulk modulus (B_{B3} = 0.36 Mbar, B_{B1} = 0.58 Mbar) and its pressure derivative (B_{B3}' = 4.80 Mbar, B_{B1}' = 5.10 Mbar), the phase transition pressure from B_3 to B_1 structure (8.64 GPa), the elastic constants with Mbar units (C_{11} = 0.472 , C_{12} = 0.310 , C_{44} =0.232) for B_3 structure, and (C_{11}= 0.451 , C_{12} =0.307 , C_{44} = 0.185) for B_1 structure, The Zener anisotropy factor A (2.86), Poisson's ratio ν (0.31), Young's modulus Y(40.03), the direct band -gap energy (E_g = 2.96 eV) in B_3 structure and the Zener anisotropy factor A (3.99), Poisson's ratio ν (0.37), Young's modulus Y(42.92), the indirect band-gap energy (E_g = 2.54 eV) in B_1 structure and the band structures are compared with the available experimental and the other theoretical results. We have, also, presented the pressure dependent behaviours of the elastic constants, graphically, for the same compound.

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