Theoretical investigation of structural, electronic and thermodynamic properties of CrO_2compound.

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Abstract

The structural, electronic and thermodynamic properties of CrO_2 compound have been performed by first-principles density functional calculations using the full linearized augmented plane wave (FP-

LAPW) method as implemented in the WIEN2k code. We employed the local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange-correlation (XC) potential. Also,we have used the Engel-Vosko GGA formalism, which optimizes the corresponding potential for band structure and density of states. Ground state properties such as the lattice parameters (a,b and c), bulk modulus B and its pressure derivative B`, have been directly calculated and compared to previous experimental and theoretical results when available. The energy gaps obtained using (EV-GGA) approximation are in reasonable agreement with experiment.

Finally, by using a quasi-harmonic Debye model, thermodynamic properties is also calculated and analyzed. The effect of temperature and pressure on the bulk modulus, volume and heat capacities are discussed.

Keywords: DFT; FP-LAPW; EV-GGA; electronic structure ; heat capacity