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HEIGHT PRESSURE EFFECT ON STRUCTURAL, ELASTIC VIBRATIONAL AND THERMODYNAMIC PROPERTIES OF CHALCOPYRITE CDGEP$_2$ FROM FIRST PRINCIPLES CALCULATIONS

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ABSTRACT

The structural, vibrational, elastic and thermodynamic properties of the chalcopyrite structure $CdGeP_2$ under pressure have been investigated by first principles calculations in the frame of the density functional theory (DFT). The obtained lattice parameter and bulk modulus under zero pressure and zero temperature are in excellent agreement with the available experimental data and other theoretical results. The phonon dispersion spectra and the obtained elastic constants shows that the $CdGeP_2$ compound is mechanically and dynamically stable up to 10 GPa and no evidence of any phase transition. The pressure dependences of the elastic constants C_{ij}, bulk modulus B, shear modulus G, Young's modulus E, Poisson ratio ν and compressibility K of $CdGeP_2$ are also successfully obtained and discussed. In addition, the thermodynamic properties of $CdGeP_2$, such as Helmholtz free energy F, internal energy E, entropy S and The heat capacity C_V are predicted by the quasi-harmonic approximation.

Keywords: Elastic properties; vibrational properties; Thermodynamic properties; high pressure; quasi-harmonic approximation.