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Structural investigation of $Si_{0.5}Ge_{0.5}$ alloy for optoelectronic applications: Ab initio study

Abstract

The structural, electronic and optical properties of the binary silicon-germanium alloy have been investigated using the projector augmented-wave (PAW) calculations with a powerful VASP package (Vienna ab initio simulation package). The structural properties of $Si_{0.5}Ge_{0.5}$ alloy have been calculated using total energy calculations and compared with our empirical model of bulk modulus. The electronic band structure and density of state of $Si_{0.5}Ge_{0.5}$ alloy show that the conduction band minimum (CBM) is located at the X point and the valence band maximum (VBM) is located at the η" point, resulting in indirect (η-X) energy band gap of 0.48 eV. The results of the refractive index and optical dielectric constant of $Si_{0.5}Ge_{0.5}$ alloy are also obtained. The PAW's results are in good agreement with experimental, theoretical and our model results.

Keywords

Bulk modulus; GeSi alloy; Modelling; Projector augmented-wave