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(Research Article)
Investigation of phononic and thermal properties of InP by using pseudopotential method

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Abstract

In this paper, according to the density functional theory and semiharmonic approximation and solving kohen's equations using plane wave, band structure, phonon scattering; Dielectric tensor, Bourne effective charge, Raman cross-section; We calculated the infrared and specific heat capacity of indium phosphide in two-phase structures on zincblend (ZB) and salt rock (Rs). The results show that this compound is more crystalline and stable in the Zb phase. Examination of phonon modes shows the existence of IR modes in both phases. Also, the effective boron charge values are close to the nominal ion values, which indicates the ion bond in this system. The calculated phonon spectrum shows a frequency gap in the range of 1179 to 288 cm^{-1}, which will be fully reflected in this range. Also, the specific heat capacity at high temperatures is close to an asymptotic value that is highly consistent with experimental results.

Keywords: InP, Dielectric tensor, Phonon spectrum, Semi-harmonic approximation, Specific heat.

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