

(Research Article)

Calculation of structural and phononic properties of LaLi_3Sb_2 compound using pseudopotential method

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Abstract

In this paper, structural parameters such as lattice constants, bulk modulus, derivative of bulk modulus, also phonon properties and density of phonon states of LaLi_3Sb_2 composition with trigonal crystal structure (space group p31m) have been discussed. The calculations have been done in the framework of the density functional theory and with the pseudopotential method in the Local Density Approximation (LDA) by the Quantum Espresso Software. The value of the bulk modulus, obtained in the LDA approximation is equal $B = 49$ GPA. The phonon spectrum of LaLi_3Sb_2 composition shows that 50% of the branches are located in the frequency range of $0\text{-}140\text{ cm}^{-1}$, which includes both optical and acoustic modes, and there is not any frequency gap observed in this range. At higher frequencies, only optical mode and frequency gap were observed. The examination of the phonon density of states showed that the heavy atoms, La and Sb only play a role in low frequencies and have no effect in high frequencies, where only the optical mode were observed, but Li atom plays a significant role in all frequencies, especially high frequencies.

Keywords: Quantum espresso, Phonon mode, bulk modul, Phonon density of states, LDA approximation.

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