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(Research Article)
Calculation of structural and phononic properties of $LaLi_3Sb_2$ compound using pseudopotential method

H. Salehi*, M. Azizi
Department of Physics, Faculty of Science, Shahid Chamran University of Ahvaz

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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 0-140 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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* Corresponding author E-mail: salehi_h@scu.ac.ir