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Theoretical investigation of the elastic and structural properties of the $LaLi_3Sb_3$ compound by the pseudo-potential method

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In this research, the structural and elastic constant properties of the $LaLi_3Sb_3$ compound, with a trigonal crystal structure (space group p31m) have been discussed [1]. The calculations have been done in the framework of the density functional theory and with the pseudo-potential method in the generalized gradient approximation (gga) by the quantum espresso software [2], and further, the elastic constants were investigated based on the density functional theory. Elastic constants give information about the hardness, stability, ductility, and brittleness of compounds. Moreover, obtaining the elastic constants subsequently gives information about elastic properties such as volume modulus B, shear modulus G, Young's modulus, and Poisson's ratio. Therefore, studying elastic constants is a functional and fundamental tool to understand the physical, chemical, and mechanical properties of the structure and can be used as a measure criterion of the resistance of a crystal to an externally applied stress. The amounts of bulk modulus B = ([40.8]) G, Young's modulus = ([80.7]) GPa and shear modulus = ([34.5]) GPa have been obtained. The value of Poisson's ratio ν=([0.17]) has been obtained for this crystal structure, which indicates the existence of a covalent bond between the two atoms. The Poisson's ratio is in the range of [(0. 1-0.25)] among solids implies the presence of a covalent bond [3]. The structure of this compound shows a small and indirect band gap between L and Γ, and also the examination of the partial density of states determined that the maximum contribution of the conduction band is related to the d orbital of the La atom and in the valence band is related to the p orbital of the Sb atom and the d orbital of the La atom. In this work, the elastic properties of this compound have been investigated for the first time.

Keywords: Band structure, $LaLi_3Sb_2$, DFT, Elastic calculations

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