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First-principles prediction of the structural, elastic, thermodynamic, electronic and optical properties of Li4Sr3Ge2N6 quaternary nitride

O. Boudrifa, A. Bouhemadou, N. Guechi, S. Bin-Omran, Y. Al-Douri, R. Khenata

Abstract: Structural parameters, elastic constants, thermodynamic properties, electronic structure and optical properties of the monoclinic Li4Sr3Ge2N6 quaternary nitride are investigated theoretically for the first time using the pseudopotential plane-wave based first-principles calculations. The calculated structural parameters are in excellent agreement with the experimental data. This serves as a proof of reliability of the used theoretical method and gives confidence in the predicted results on aforementioned properties of Li4Sr3Ge2N6. The predicted elastic constants Cij reveal that Li4Sr3Ge2N6 is mechanically stable but anisotropic. The elastic anisotropy is further illustrated by the direction-dependent of the linear compressibility and Young's modulus. Macroscopic elastic parameters, including the bulk and shear moduli, the Young's modulus, the Poisson ratio, the velocities of elastic waves and the Debye temperature are numerically estimated. The pressure and temperature dependence of the unit cell volume, isothermal bulk modulus, volume expansion coefficient, specific heat and Debye temperature are investigated through the quasiharmonic Debye model. The band structure and the density of states of Li4Sr3Ge2N6 are analyzed, which reveals the semiconducting character of Li4Sr3Ge2N6. The complex dielectric function, refractive index, extinction coefficient, absorption coefficient, reflectivity and electron energy-loss function are calculation for incident radiation polarized along the crystallographic directions and for energy up to 40 eV.

Keywords : Quaternary nitride, First-Principles calculations, Elastic constants, Electronic structure, optical properties, Thermal Properties