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(Research Article)
Investigation of structural, phononic and thermodynamic properties of sodium sulfide compound in the cubic phase (zinc-blend) using pseudopotential method

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Abstract

In this paper, the structural, phononic and thermodynamic properties of sodium sulfide compound in the cubic phase (zinc-blend) have been studied. The calculations were done using the ultrasoft pseudopotential method in the framework of the density functional theory and using the Quantum Espresso software using the generalized gradient approximation (GGA). The value of lattice constant and volume modulus after optimization were obtained as 6.18 Angstroms and 1.15 Gigapascals, respectively, then by calculating the phonon scattering, we get the scattering diagram with 6 phonon branches in the symmetrical direction W-L-Γ-X-W-K. and we noticed the existence of a frequency gap from 101.19 to 226.58 Hz in the scatter diagrams and also the examination of the thermal properties show that the heat capacity of the compound present in the zinc blend phase at low temperatures according to experience is proportional to the third power of the temperature and reaches a saturation value at high temperatures, which indicates that it is no longer dependent on temperature.

Keywords: Quantum Espresso, Sodium sulfide, Phononic properties, Structural properties, Thermodynamic properties.

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