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(Research Article)
Investigation of phononic, dynamic and thermal properties of indium nitride in different phases

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Abstract

In this paper, the phonon, dynamic and thermal properties of indium nitride in two phases are investigated. The calculations are performed using the pseudopotantial method in the framework of density functional theory and by using the quantum-espresso Package. In the calculations, the exchange-correlation terms of LDA, GGA and PBE0 approximation are used. Investigation of phononic properties shows that in this combination in the two phases Wz and Zb there is a frequency gap. From the study of thermal properties we find that the heat capacity drop is at low temperatures is as follos T^3. At high temperatures, the heat capacity is also close to the Dulan-Petty law.The results from the phonon spectrum indicate that from the frequency of 209. 885 to 453 .112 cm $^{-1}$ there is no acoustic and optical phonon modes and the most stable phase; Phase is the Wz.

Keywords: Density functional theory, Indium Nitrid, Frequncy gap, Phononic mode.

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