Journal of Acoustical Engineering Society of Iran, Vol. 10, No. 1, 2022

(Research Article)
Calculation of phononic and thermal properties of the CaB_2 using the perturbation density functional theory

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Received: 2022/01/29, Accepted: 2022/09/14
DOR 20.1001.1.23455748.1401.10.1.8.7

Abstract

In this paper, the phononic structure and Enthalpy of CaB_2 compound in simple hexagonal and orthorhombic OsB_2 phase have been investigated. The calculations were performed using the pseudo-potential method in the framework of the density functional theory and using the Quantum-Espresso code. Using the group theory and the characteristic table of the composition point group, the phonon modes were identified in terms of symmetry species. Phonon modes are obtained at points with high symmetry in both phases, which are all positive, so they do not show structural instability. Also, it can be seen that the frequency of acoustic phonons becomes zero when their energy tends to zero, while optical phonons have a repulsive frequency of zero and are almost without scattering. In addition, the enthalpy diagram in two phases shows the heat absorbed by the system. The obtained results are in good accordance with other available data.

Keywords: OsB_2, Enthalpy, Phonon structure, CaB_2.

pp. 74-80 (In Persian)

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