Journal of Acoustical Engineering Society of Iran, Vol. 9, No. 2, 2022

(Research Article)
Investigation of the phononic and thermal properties of tungsten disulfide compound using density functional theory

N. Zhulayi Bakhoda, H. Salehi*
Department of Physics, Faculty of Science, Shahid Chamran University of Ahvaz

Received: 2021/02/28, Accepted: 2021/08/19

Abstract

In this paper, the phononic and thermal properties of tungsten disulfide have been studied. The aim of this study was to investigate the phonon and thermal properties such as heat capacity and enthalpy. The calculations are performed within the framework of density functional theory by pseudo-potential methood and by Quantum Espresso computational package and their exchange-correlation function is of LDA and GGA type. From the study of thermal properties, we find that the drop in heat capacity at low temperatures is T^3. At high temperatures, the heat capacity approaches ($3NK_B$ =71.673J / K.mol Dulong-Petit law). Also, the specific heat value and entropy of this compound at room temperature were 65.221 J / K.mol and 68.757 J / K.mol, respectively. In the phonon scattering diagram, 3 Acoustic branches and 15 optical branches were obtained. Also, the phonon scatter diagram and the density of phonon states were compared in terms of state matching. The results obtained are consistent with other available data.

Keywords: Tungsten disulfide, Density functional theory, Phonon modes, Heat capacity.

pp. 1-8 (In Persian)

* Corresponding author E-mail: salehi_h@scu.ac.ir

[DOR: 20.1001.1.23455748.1400.9.2.2.6]