First-principles investigation of the electronics, optical, mechanical, thermodynamics and thermoelectric properties of Na based Quaternary Heusler alloys (QHAs) NaHfXGe (X = Co, Rh, Ir)

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Abstract

In this study, we explored the electronic and thermoelectric (TE) properties of the Na-based Quaternary Heusler Alloys (QHAs) NaHfXGe (X = Co, Rh, Ir) using density functional theory (DFT). We performed the spin-polarized DFT calculations at the general gradient approximation (GGA) level and confirmed the ground state non-magnetic configuration of NaHfXGe. The mechanical and thermodynamical stabilities are analyzed and discussed to validate the stability by calculating the elastic constant and phonon dispersion curve. A thorough investigation on the electronic properties are carried out by performing the GGA, GGA+U, and GGA+SOC formalism where we report the semi-conducting characteristic of NaHfCoGe and NaHfRhGe QHAs. However, NaHfIrGe is predicted to be a non-magnetic metal. From the calculated optical properties we found that the most active optical absorption occurs within the vis–UV region with

10^5 cm^{-1}, therefore the studied QHAs are proposed to be a promising optoelectronic materials. The results of the thermodynamic properties have shown that NaHfXGe follows Debye's low-temperature specific heat law and the classical thermodynamics of the Dulong-Petit law at high temperatures. The calculated TE efficiency using GGA+SOC formalism at T = 1200 K are ZT∼1.22 and 0.57 for NaHfCoGe and NaHfRhGe, suggesting that these materials are potential TE materials to operate at high temperature.