Abstract

First-principle calculations were carried out to demonstrate the structural, electronic, thermoelectric and thermodynamic properties of ternary $NaXN_2$ (X=W,Rh,Os) nitrides by utilizing density functional theory with Perdew-Burke-Ernzerhof Generalized- Gradient Approximation as exchange and correlation functional. Theoretical calculations of ternary $NaXN_2$ (X=W,Rh,Os) nitrides, such as electronic band structure and density of states (DOS) were performed. The partial density of states (PDOS) was also included to determine the contribution of individual atoms to the electronic states. The theoretical data reveal the metallic nature of ternary $NaXN_2$ (X=W,Rh,Os) nitrides, exhibiting band gap values of 0.0 eV. Thermoelectric properties are calculated using Boltztrap2 code. To evaluate the transport performance of compounds at different temperatures, thermoelectric (TE) properties such as power factor (PF), Seebeck coefficient (S), thermal conductivity (k/τ), electrical conductivity (σ/τ), power factor, and figure of merit (ZT) is established. Results reveal that, $NaXN_2$ (X=W,Rh,Os) exhibit maximum ZT values up to 0.74, 0.028 and 0.00002, respectively. High figure-of-merit ($ZT = 0.49$) of $NaWN_2$ at room temperature) reflects its suitability to use in thermoelectric systems. The estimated thermodynamic properties, provides the thermodynamic stability of $NaXN_2$ (X=W,Rh,Os) nitrides by using Gibbs2 code. Hence, these properties indicate that $NaXN_2$ (X=W,Rh,Os) nitrides have great potential for use in energy storage and thermoelectric devices.