Abstract:

Energy crisis is a global issue and researchers are putting a lot of effort into arranging new sources. Hydrogen is a potential candidate as an alternate fuel with its characteristics of; low cost, non-toxicity and renewable nature. The main challenge behind the usage of hydrogen is its hazardous nature while its storage in gaseous or liquid state. The scientists are looking for new compounds such as metal hydrides for a safe storage of this valuable fuel. In this work we have proposed and investigated new compounds; K2ZnH4, Rb2ZnH4 and Cs2ZnH4 as metal hydrides and checked for their stability using Density Functional Theory. The compounds were found stable in the orthorhombic phase. The evaluated elastic constants, and their analyses pointed that K2ZnH4 and Rb2ZnH4 are mechanically stable, while Cs2ZnH4 is unstable, as per Born stability criteria. The electronic properties were studied for the calculation of bandgap and density of states. The compounds were found showing semiconductor nature with direct bandgap. Thermoelectric properties were evaluated using BoltzTrap code like electrical conductivity, thermal conductivity, specific heat capacity, Seebeck coefficient and Hall coefficient. The calculated results show that electrical and thermal conductivities increase with carrier concentration. Overall, theoretically, we propose novel solid-state hydrides; K2ZnH4 (with Gravimetric Hydrogen Density (GHD) as 2.73 wt.%), Rb2ZnH4 (1.67 wt. %) and Cs2ZnH4 (1.20 wt. %) using first principles calculations.