Abstract

Hydrogen storage is appealing to research interest as it has green, renewable, and clean energy properties. So, frequently research has been conducted to find innovative and suitable materials that meet the criteria of H_2 storage. First-principles study of XPH_2 (X=Li, Na, K) and $XPdH_3$ (X=Li, Na, K) compounds are conducted to examine their properties by using WEIN2k code. Structural, thermoelectric, elastic, and electronic properties of these metal hydrides have been studied. The gravimetric hydrogen capacities of XPH_2 (X=Li, Na, K) are 5.048, 3.6011, and 2.796 respectively. The structural properties of these compounds show the tetragonal nature of XPH_2 (X=Li, Na, K). The electronic properties of these compounds show the metallic nature of these compounds. The gravimetric hydrogen capacities of $XPdH_3$ (X=Li, Na, K) are 2.598, 2.2381, and 2.0355 wt % respectively. The structural properties of these compounds show the cubic nature of $XPdH_3$ (X=Li, Na, K). The mechanical properties of these six compounds show that XPH_2 (X=Na, K) and $XPdH_3$ (X=Li, Na, K) hydrides satisfied Born stability criteria, and are stable but $LiPH_2$ is not mechanically stable. Besides, different thermodynamic properties like heat capacity at constant pressure and volume, Debye temperature, entropy, and free energy under elevated temperature and pressure conditions are investigated using the GIBBS2 code.