Abstract

In recent years, hydrogen storage obtained is attractive in research interests due to the clean, renewable and green energy properties of hydrogen and its usage as energy source. However, many researches occurred frequently in order to find suitable and innovative material that fulfill the criteria of hydrogen storage materials. Therefore, this research is also focused on the aim of finding suitable hydrogen storage material. In this research, $ZrCoH_3$, $ZrNiH_3$ and $ZrCuH_3$ compounds are theoretically studied to find out their hydrogen storage properties. First principle calculations are carried out through density functional theory in CASTEP code. Structural, mechanical, electronic, optical and thermodynamic properties of these materials have been studied. Although, these materials used for hydrogen storage purpose therefore, their gravimetric hydrogen storage densities also calculated. All of these compounds have orthorhombic crystal structure. Moreover, mechanical properties of the studied compounds such as bulk, shear and young's moduli, Poisson's ratio and Vickers hardness have been reported and proved their mechanical stability by satisfying Born stability criteria. Their dynamic stability behavior proved through phonon dispersion curves which obtained through density functional perturbation theory.