Abstract

The increase in demand for clean and green energy sources has compelled scientists to work on renewable and sustainable power resources. Hydrogen possesses substantial energy potential but is too dangerous to use directly because of its extremely explosive nature, and its storage remains a challenge, which limits its use. One of the schemes is to store the hydrogen in compound form as hydrides. Using first-principles calculations, we studied a novel perovskite compound(s) in the form of **$XBeH_3$ (X = Ag, Cd, In)**. The investigated compounds; $AgBeH_3$, $CdBeH_3$, and $InBeH_3$ were found stable in simple cubic structures with lattice constants as 3.42, 3.57, and 3.64 Å respectively. The ductility of $AgBeH_3$ and $CdBeH_3$ hydrides, as well as the brittleness of $InBeH_3$, are consistently demonstrated by Cauchy's pressure and the bulk-to-shear modulus ratio (B/G). According to the study of their electrical characteristics, all compounds show metallic characteristics. The mechanical and thermodynamic stabilities were observed in the $XBeH_3$ perovskites. The hydrogen storage capacities measured by gravimetric analysis for $AgBeH_3$, $CdBeH_3$, and $InBeH_3$ are 2.54, 2.42, and 2.38 wt%, respectively. The temperatures at which $AgBeH_3$, $CdBeH_3$, and $InBeH_3$ desorb hydrogen are 413.4, 346.9, and 406.9 K, correspondingly. Our results indicate that $AgBeH_3$ hydrides were found better for hydrogen storage among the family due to their better thermodynamic, gravimetric, and mechanical properties.