Abstract

Developing sustainable energy solutions is made possible by the falling prices of renewable energy. Renewable energy's unstable nature, meanwhile, continues to be a significant barrier. A high density storage option for renewable energy can be hydrogen (H_2). The potential for various potential applications in hydrogen storage was increased by the cubic transition metal hydride frameworks. This research focuses on the theoretical study of metal hydrides $LiXH_3$ (where X = Ti, Mn, and Cu). To explore the structural electronic, thermoelectric, and hydrogen storage gravimetric values of the perovskite type hydrides $LiTiH_3$, $LiCuH_3$, and $LiCuH_3$ using first principles calculations as part of the investigation. Under the umbrella of DFT, the FPLAPW method and GGA perturbation, which are now used for Wien2k-code, have been implemented. The electrical, structural, and thermoelectric properties' computed parameters are in agreement with the literature results. $LiCuH_3$ is more stable than $LiMnH_3$ and $LiTiH_3$, based on the optimization graph. The merging of valence and conduction bands at the fermi level in the band structure reveals a metallic structure. Mostly contribution of electronic states for the TDOS are provided by the d-states of the atoms named as titanium, manganese, and copper. The hydrogen storage capacity of the materials $LiTiH_3$, $LiMnH_3$, and $LiCuH_3$ are determined that have gravimetric storage ratios of 5.22%, 4.66%, and 4.11%, respectively. According to their temperature-dependent thermoelectric properties, all the materials under study were able to absorb heat energy, which further proves their high electrical and thermal conductivity. According to our research, the investigated compounds show potential for efficiently storing hydrogen molecules and could be used as some world's best hydrogen storage materials.