The global community is currently grappling with two significant challenges: climate change and the depletion of non-renewable power sources. To address these issues, scientists are paying increased attention to hydrogen as a potential alternative energy carrier, as it is both ecologically favorable and has the potential to replace non-renewable energy sources. However, scientists face difficulties in storing and transporting hydrogen directly. Perovskite hydrides have gained considerable interest as they exhibit excellent ion exchangeability and high gravimetric hydrogen storage capacity. This study specifically examines the hydrogen storage capabilities of $NaAlO_{3-x}H_x$ perovskite using the famous DFT-based CASTEP simulation code. The research reveals that after hydrogen was inserted into the pristine material, the material's cubic structure along with lattice parameters manifests variation. The study also reveals that the hydrogen-incorporated compositions were structurally and thermodynamically stable, with Born's mechanical stability criteria being fulfilled by all compositions. The ductile or brittle nature of the compounds varied with the amount of hydrogen inserted, as shown by Cauchy's pressure and Poisson's ratio. Additionally, the continuous insertion of hydrogen into the pristine material significantly impacted the electronic states, as demonstrated by the density of states and plots of band gap. After the complete insertion of hydrogen, the band gap fell from 5.86 eV to 0 eV, making the final compound metal, it also affects the material's optoelectronic properties. This research provides detailed insights into optical parameters such as absorption, reflectivity, complex dielectric function, and energy loss function. The gravimetric storage capacity of the material increased from 0.32wt% to 5.4wt% after inserting 100% hydrogen into it. $NaAlH_3$ is determined to be an excellent material for hydrogen storage based on our conclusions.