Abstract

Hydrogen storage has emerged as a compelling avenue for scientific inquiry and research due to its unparalleled efficiency as an energy supply, rendering it a promising candidate for future examination. The present study used the GGA-PBE methodology, which is accessible through the CASTEP program, to examine the perovskite $K\square\square3-\square\square\square$. The present study examines the impact of various substituent concentrations (x = 0, 0.3, 0.6, 0.9, 1.2, 1.5, 1.8, 2.1, 2.4, 2.7, and 3.0) on the structural, electrical, optical, and mechanical properties of the perovskite $K\square\square3-\square\square\square$ hydride material in the context of hydrogen storage applications. Based on the analysis of elastic constants, it is evident that the structure exhibits perfect stability and is capable of being synthesized. Furthermore, the brittleness of these hydrides is evidenced by the measurements of Cauchy pressure and Pugh's ratio. Furthermore, the mechanical properties exhibited the stability of both compounds, both before and after the process of hydrogenation. The reduction in brittleness and anisotropic factor is observed when hydrogen content is substituted for oxygen, resulting in increased ductility of perovskite films. The introduction of additional hydrogen resulted in a decrease in the band gap from 4.66eV to 2.763eV. The decrease in band gap leads to the emergence of semiconductors with indirect magnetic properties. This observation suggests that the use of hydrogen as a dopant material in perovskite hydride will result in an improvement in electronic characteristics. The enhancement of dopant concentration renders it more appropriate for utilization in optoelectronics applications. The compounds being studied are subjected to optimization methods in the cubic phase, resulting in the determination of optimal lattice constants of 4.83 for KSrH3. The introduction of hydrogen resulted in a transformation of the structure from a cubic configuration to a deformed or pseudo-cubic configuration. The determination of gravimetric hydrogen storage capacity for KSrO3 and KSrH3 has been achieved through an investigation of their intrinsic hydrogen storage features. The gravimetric value of material KSrH3 is determined to be 2.628%. The presence of hydrogen (H) enhances the optical characteristics of these materials, rendering them suitable for use in hydrogen storage and transportation within the industry..