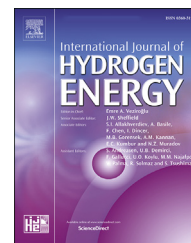


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Efficient hydrogen storage in KCaF_3 using GGA and HSE approach

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HIGHLIGHTS

- Hydrogen storage characteristics were improved via H-inclusion.
- Band engineering was performed utilizing both GGA and HSE03 formalisms.
- Redshift of energy states was noticed for all studied materials.
- Direct bandgap was achieved mainly for a new end material KCaH_3 .
- Brittle nature is observed for all substituted materials.

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ABSTRACT

Being a renewable and sustainable energy carrier, hydrogen energy has garnered great interest having some technical barriers related to storage aspects. Hydride materials exhibit potential hydrogen storage capacities efficiently and safely. The current study has been performed in the framework of density functional theory to examine structural and optoelectronic properties of $\text{KCaF}_{3-x}\text{H}_x$ ($x = 0, 0.6, 1.2, 1.8, 2.4$, and 3) compounds to understand their contribution about hydrogen storage. The mechanical stability of these compounds with elastic constants and negative formation enthalpies suggests these materials are stable and synthesizable. Insertion of impurity into pristine material led to an increase in optimized lattice parameter from 4.31 to 4.48 Å where no previous study is available to compare lattice constants other than pristine KCaF_3 that is well consistent with existing literature. Computed and plotted results of plastic properties for different H-inclusions manifestly depict a decrease in elastic moduli, anisotropic and brittle nature of all studied materials. The density of states and band diagrams were drawn utilizing both GGA and HSE03 formalisms, where observations manifest not only an upsurge in bandgap but also shifting from indirect to direct nature. Two effects Burstein-Moss shift and bandgap renormalization were explored to investigate the shifting of absorption edge toward the valence band that results in bandgap narrowing. Optical parameters were also well explained within the photon energy range of 0 – 35 eV. Startling results of absorption spectra reveal prominent redshift increases in the UV region. Among all H-inclusions high value of the static refractive index ($n(0) = 3.77$) and dielectric function with minimum absorption losses possess KCaH_3 only appropriate material for storage aspects. Also,

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