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Structural stability and electronic structures of $YH_2.83$ and $ScH_2.83$

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$YH_{2.83}$ and $ScH_{2.83}$ are a defected system in which some interstitial sites of hydrogen atoms are void. We used \textit{ab-initio} method to study their structural stability and electronic structures. The hcp phase of YH_3 and ScH_3 is used as an initial structures, which composes of 6 metal atoms and 18 H atoms per unit cell. Then, $YH_{2.83}$ and $ScH_{2.83}$ are obtained by removing one of H atoms from the unit cell. The results show that they are dynamically stabilized but not energetically favorable. Their energy gaps are closed by the crossing of the valence band maximum crossing at the Fermi level.

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