Computational study of the Dehydrogenation Effect of Dopant Ti on Nanostructured NaAlH4 Cluster

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September 28, 2020

Abstract

Employing the evolutionary algorithm combined with density functional theory and perturbation theory model, we investigate the geometric and electronic structures of pure and Titanium-doped Na4Al4H16 cluster to demonstrate the effect of dopant Ti on the dehydrogenation properties of the nanostructured NaAlH4. The result shows the Ti-doped Na4Al4H16 clusters are more stable thermodynamically, but the average dehydrogenation enthalpies and the energy barriers for H2 desorption are significantly decreased. Doping of Ti weakens the Al-H bond, reduces the dehydrogenation temperatures, and the dehydrogenation performance of the NaAlH4 nanocluster is conspicuously promoted.

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