Lithium decorated C3N as high capacity reversible hydrogen storage material: Insights from density functional theory simulations

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Abstract

Lithium-decorated (Li-decorated) C3N has been investigated as a potential material for high capacity reversible hydrogen storage. The energetic stability, dynamical stability and thermal stability were studied, indicating that C3N is energetically stable, imaginary frequencies are not found from the result of phonon spectrum calculation, and the free energy vibrates slightly around -64.63 eV during the 5000 fs period and no structure reconstruction. Electronic properties showed the band gaps are 0.39 eV and 1.12 eV, via PBE and HSE calculations, respectively. The four probable Li-adsorbed sites were calculated, indicating that the hollow site above the center of a hexagon ring HC site is the most likely site to absorb Li atom. Hydrogen molecules were added one by one to research the maximum hydrogen gravimetric density. Each Li atom can attach 10 hydrogen molecules within the range of physical adsorption processes (-0.1 ~ -0.4 eV/H2) and the hydrogen storage capacity can reach 8.81 wt%. Li-decorated C3N shows the greatest potential for on-board reversible solid-state hydrogen molecule storage application.

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