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The effects of Li adatoms on defected graphane: A first-principles study

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Abstract content
   (Max 300 words)
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Using density functional theory (DFT), we study the energetics, electronic and magnetic properties of lithium (Li) adatom on the hexagonal, bridge and vacancy sites of graphane. We find that Li is most thermodynamically stable on the vacancy site.The incorporation of Li enhance strong spin polarized states within the band gap of graphane, due to notable hybridization between Li-1s and C-2p states. Li on defected graphane exhibits half-metallic character with a magnetic moment of 2 Bohr magneton in the ferromagnetic states. Moreover, our calculated magnetic moment is mainly dominated by Li-1s and C-2p states. Lithium adatom on defected graphane is found to play an important role of defects in semiconductor which facilitate the tunability of the bandgap and also influence the magnetic ordering of localized states on the vacancy site.

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