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Enhancement of Li and graphane interaction through extended H vacancy pathways for Li-ion batteries: Ab initio study

First-principles density functional theory calculations were performed to study the energetic stability, electronic and electrochemical properties of Li atoms on the H vacancies (VH) in graphane. On a single VH, Li relaxes to a height (dLi-C) of 2.07Å with a binding energy (Eb) of 1.82eV/Li. The obtained Eb value is more than the Li standard bulk cohesive energy of 1.63eV suggesting a possible uniform dispersion of Li atoms with less clustering on the graphane sheet. The modulation of VH (VH1(L), VH2(L), VH3(L), VH4(L) and VH5(L) refer to one, two, three, four and five VH along the line pathway) increases the Li binding energy from 1.82eV/Li for VH1(L) to 2.92eV/Li for VH5(L). Furthermore, multiple Li atoms were adsorbed on top of VH1(L), VH2(L), VH3(L), VH4(L) and VH5(L) and the high binding energies of 1.82eV/Li, 1.68eV/Li, 1.78eV/Li, 0.94eV/Li and 1.48eV/Li were obtained. These values are still comparable to the standard cohesive energy of Li in its stable form, suggesting its inability to form undesirable clustering. A transition from insulator to metallic behavior was observed with introduction of Li new states around the fermi level. For VH5(L), a storage capacity of 207.49 mAh/g was obtained comparable to other promising 2-dimensional anode materials.

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