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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) following a Line pathway as well as the zigzag pathway on a graphane sheet for LIBs. The results of Li on a single H vacancy VH1(L) revealed that it successfully induced interaction based on the improved binding energies, charge transfer and significantly shortened Li height, as compared to those of pristine graphane. An increase in H vacancies along the line pathway from one VH1(L) to five VH5(L) leaves behind localized electrons ready to interact with the Li atom resulting in high binding energies ranging from 1.82eV to 2.92eV. While creation of H vacancies along the zigzag pathway from one VH1(Z) to five VH5(Z) leaves behind electrons that pair and repel Li atom away yielding undesired low binding energies which become a setback for LIBs. For the increment of Li content following a line VH pathway, the binding energies of Li on configurations VH1(L) to VH5(L) tend to reduce in order, endearingly are still higher than the minimum Li standard bulk cohesive energy of 1.63 eV, suggesting a possible uniform dispersion of Li atoms with less clustering on the graphane sheet. A transition from insulator to metallic behaviour was observed with induced new Li states at the vicinity of the fermi level, which will enhance electron transmission in the graphane sheet. At five Li content adsorbed along the line configurations, a relatively high storage capacity of 207.49 mAh/g with its corresponding lithiation potential of 1.48 V are achieved and are comparable to the other previously studied 2-dimensional anode materials with high Li concentration.

Keywords: graphane, Li-ions batteries, adsorption, binding energy. 2-D anode materials, LIBs

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

Primary author: KGALEMA, Sentserere

Co-author: Dr MAPASHA, Refilwe

Presenter: Dr MAPASHA, Refilwe

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