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Li adsorption on a self-healed graphane for the next generation ion batteries.

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Density functional theory calculations were performed to study the behaviour of Li atom on self-healed various CH divacancies graphane focusing on the reconstructed lattices. The energetic stability, structural and electronic properties of different Li configurations on self constructed topological 5-9-5 and 9-5-9 defects were examined. These lithiated configurations have high binding energy significantly more than that of Li on graphene and bulk metalic lithium, suggesting a plausible materials for experimental characterizations. All the lithiated configurations relaxes towards the vacancy with 5-9-5 defect having a 0.00 Å height. The Li atom introduces delocalised states within the band gap, exhibits metallic character with considerable electronic states at the Fermi level, which can provide good electrical conductivity during the battery cycle. These results suggest that Li configurations on self constructed topological 5-9-5 and 9-5-9 defects can be utilized as a promising anode material for the application in Li ion batteries with fast charge/discharge rates.

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

No

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

N/A

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