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

Density functional theory calculations where performed to study the behaviour of Li atom on self-healed graphane, focusing on the reconstructed region. The energetic stability, structural and electronic properties of different Li configurations where examined. Li atoms prefers to strongly bind at the octagon site transferring almost of its electronic charge towards its surrounding carbon atoms based on Barder charge analysis criterion, unlike in the case of pristine. Li atom enables semiconducting-metallic transition with an induced Li states at the vicinity of Fermi level, suggesting an introduction of electronic conductivity which will enhance electron transmission in the graphane sheet. The self-healed graphane promises to be a high performance electrode material by exhibiting lithiation voltage of 1.89 V. Lastly, we found that self-healed graphane monolayer can specifically be suitable for anode material due to its calculated relative high storage capacities and high rate performance for next generation ion batteries.

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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