

Abstract Submitted  
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**Enhanced Absorption and Diffusion Properties of Lithium on B,N,V<sub>C</sub>-decorated Graphene**<sup>1</sup> MENGTING JIN, Chengdu Green Energy and Green Manufacturing Technology RD Center, LINGCHAO YU, YANNING ZHANG, University of Electronic Science and Technology of China — Systematic first-principles calculations were performed to investigate the adsorption and diffusion of Li on different graphene layers with B/N-doping and/or C-vacancy, so as to understand why doping heteroatoms in graphene anode could significantly improve the performance of lithium-ion batteries. We found that the formation of single or double carbon vacancies in graphene are critical for the adsorption of Li atoms. While the N-doping facilitates the formation of vacancies, it introduces over binding issue and hinders the Li diffusion. The presence of B takes the excessive electrons from Li and N and reduces the energy barrier of Li diffusion on substrates. We perceive that these clear insights are crucial for the further development of graphene based anode materials for lithium-ion batteries.

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Yanning Zhang  
Univ of Electronic Sci  
Tech

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