(One page abstract format: including figures and references. Please follow the model below.)

The effect of oxygen content on lithium storage in graphite oxide by first principles studies

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Abstract (Arial 10)
Nowadays, lithium ion batteries (LIBs) have been widely used in portable electronic devices, owing to their high energy densities [1]. LIBs are also considered as promising devices for electric vehicles [2]. Commercial LIBs commonly use graphite as the anode material. However, the relative low Li capacity of graphite limits the performance and hence the applications of LIBs [3]. A possible route to enhance Li storage is chemical modification of graphite by oxygen [4,5]. However, the effect of oxygen content on the performance of such anode materials is known only approximately [6]. In this work, we systematically investigated the adsorption, diffusion, and intercalation behaviors of Li ions in graphite oxide at various oxidation levels, based on density functional theory calculations. The goal is to design graphite oxide compounds with high lithium potentials, large diffusion rate for Li ions, and high Li capacity. This theoretical work will not only provide better insight into the microscopic mechanism of Li storage in graphite oxide, but also be a guidance for experimental fabrication of LIBs with improved performance.

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Figures