

New insight into lithium intercalation and doping implications at edged graphite in Lithium-Ion Battery

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Li intercalation at interface between electrolyte and graphite is an important step in lithium ion batteries and has a significant impact on battery performance. However, the edge and doping effects of graphite on Li intercalation remain elusive. In this work, based on density functional theory (DFT), two edges of graphite, the zig-zag edge and armchair edge, were comprehensively studied. Compared with the bulk of graphite, the graphite edges show a huge edge effect on Li adsorption and highly promote its adsorption. Furthermore, the adsorption energies of Li at the zig-zag edge are much higher than those at armchair edge, which results from the existence of spin electrons on the edged carbons of zigzag system. The formed unoccupied p_z orbital above the fermi level in zigzag edged system is beneficial to Li adsorption. Besides, boron and nitrogen doping at the edge were identified to change both the adsorption and diffusion behaviors of Li in the two systems, which might give some guidance of graphite modification.