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Finding out the optimal boron concentration in BC_x sheets for high capacity anode material in Li-ion batteries DEYA DAS, RAHUL HARDIKAR, Indian Institute of Science, SANG SOO HAN, KWANG RYEOL LEE, Korea Institute of Science and Technology, ABHISHEK KUMAR SINGH, Indian Institute of Science — Boron doped graphene shows better adsorption of Li compared to pristine graphene and has been investigated as a potential anode material for Li-ion batteries. Using first principles density functional theory calculations, we investigate the effect of increasing boron concentration on the gravimetric capacity of mono-layered boron doped graphene sheets, BC_x (x = 7, 5, 3, 2 and 1). Li storage capacity increases with the increase in boron concentration giving highest capacity for monolayer BC_2 ($\sim$ 1400 mAh/g), and is about 1.6 times higher than previously reported capacity of BC_3. This is due to the more number of available empty states above the Fermi level in BC_2 compared to other sheets. Moreover, owing to a very low Li diffusion barrier, the Li kinetics in BC_2 is also found to be better among all the layered boron doped carbon sheets. Further enhancement of B concentration, as in BC, leads to strong binding of Li, thereby hindering the delithiation processes. Hence, BC_2 with optimal concentration of B among the BC_x phases, emerges as a promising choice for anode material in rechargeable Li ion battery.

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