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Mono-layer BC_2 a high capacity anode material for Li-ion batteries[1] RAHUL HARDIKAR, ATANU SAMANTA, Materials Research Centre, Indian Institute of Science, Bangalore, India, SANG SOO HAN, KWANG-RYEOL LEE, Korea Institute of Science and Technology, Seoul, South Korea, ABHISHEK SINGH, Materials Research Centre, Indian Institute of Science, Bangalore, India — Mono-layer of graphene with high surface area compared to the bulk graphite phase, shows less Li uptake. The Li activity or kinetics can be modified via defects and/or substitutional doping. Boron and Nitrogen are the best known dopants for carbonaceous anode materials. In particular, boron doped graphene shows higher capacity and better Li adsorption compared to Nitrogen doped graphene. Here, using first principles density functional theory calculations, we study the spectrum of boron carbide (BC_x) mono-layer phases in order to estimate the maximum gravimetric capacity that can be achieved by substitutional doping in graphene. Our results show that uniformly boron doped BC_2 phase shows a high capacity of ? 1400 mAh/g, much higher than previously reported capacity of BC_3.

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