Supporting information

B_2C_9 as the High-performance Li-ion Battery Anode: Effects of Boron-incorporation and Strain-engineering on the Adsorption and Diffusion of Lithium

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We quantified transport in the 2D DP framework using (i) band-edge parabolic fits for effective masses, (ii) band-edge energy shifts under biaxial strain for deformation-potential constants E_1, and (iii) energy-strain fitting for the 2D elastic modulus C_{2D}. From these, we obtained carrier mobilities of Li adsorbed B_2C_9 monolayer.

Effective mass at the band edge k_0:

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}\Big|_{k=k_0}$$

Mobility (2D DP model):

$$\mu = \frac{e\hbar^3 C_{2D}}{k_B T m^* m_d E_1^2}$$

$m^*_n = 0.69\ m_0$, $m^*_p = 0.88\ m_0$;

$\mu_n \approx 1.03\times10^4\ cm^2/(V\cdot s)$, $\mu_p \approx 2.26\times10^4\ cm^2/(V\cdot s)$.