Rational design of C_3N/C_3B p-n heterostructure as a promising anode material in Li-ion batteries

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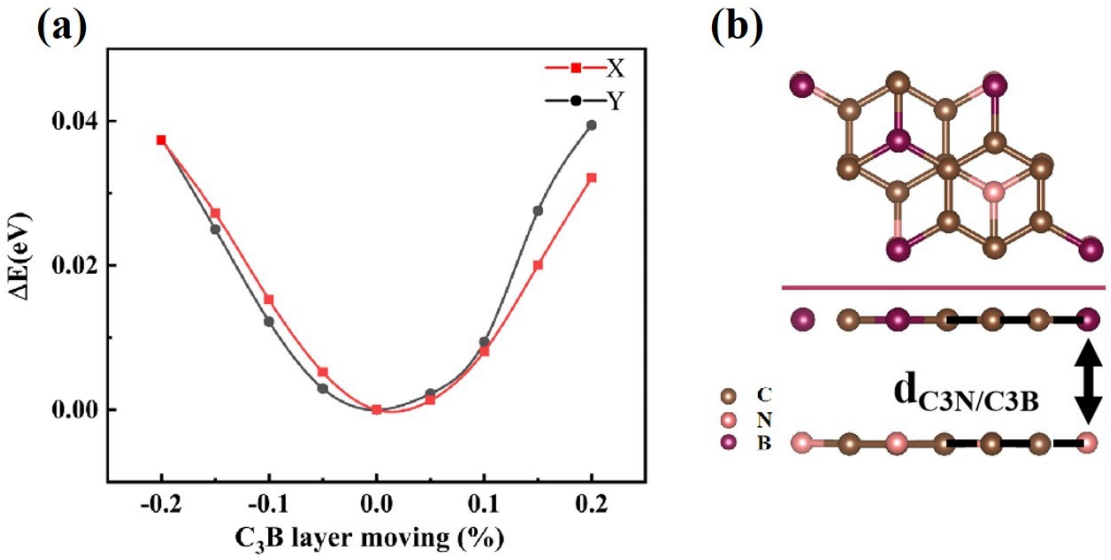

Fig. S1. (a) Energy as a function of C_3B moving relative to C_3N of C_3N/C_3B along with X and Y directions. (b)The most stable structure in which C_3B's relatively moving ratio is 0.

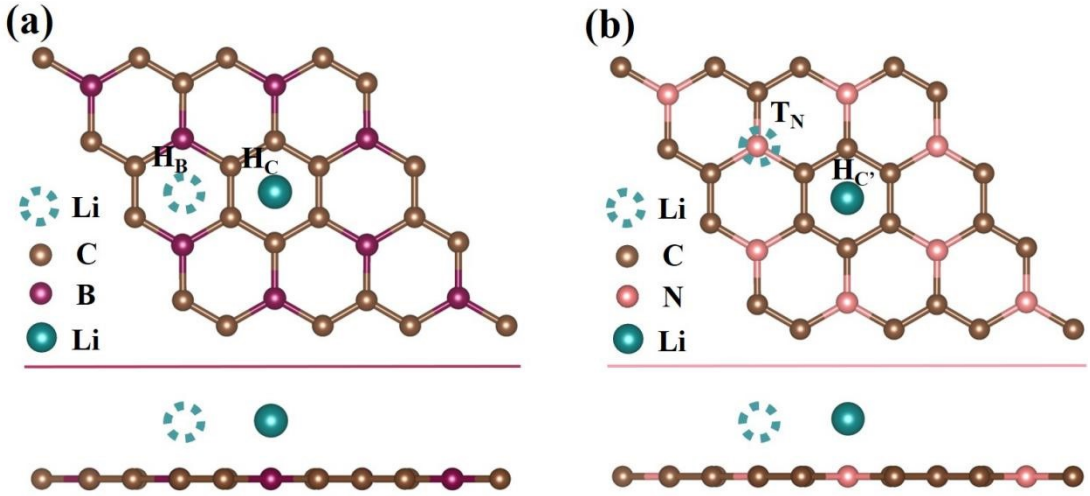

Fig. S2. Top and side views of the Li adsorption sites on the C_3B and C_3N monolayer (Li/ C_3B, Li/C_3N). H_C and H_B sites are on the C_3B, and H_C' and T_N sites are on the C_3N.

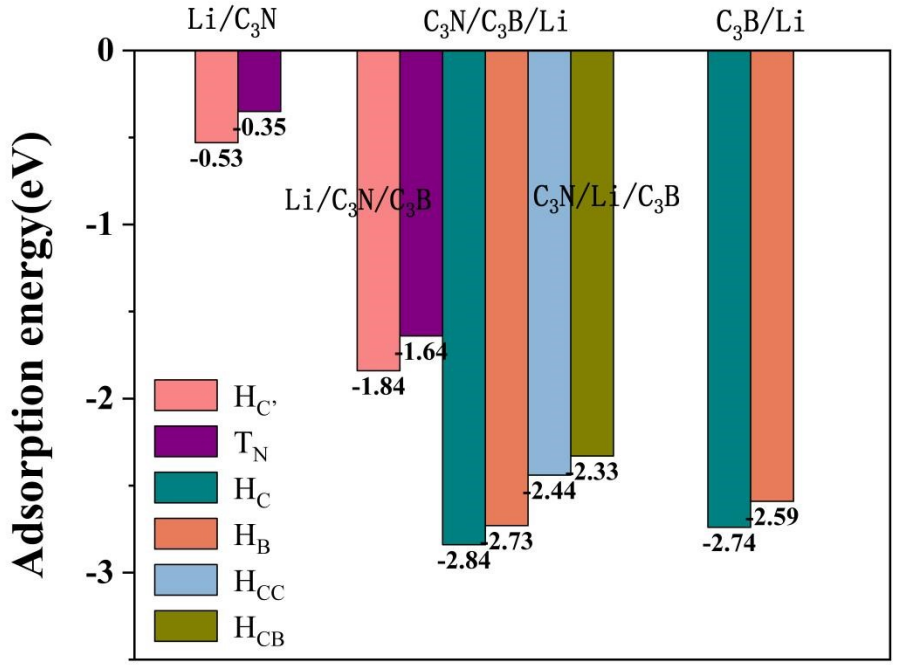

Fig. S3. The adsorption energy of Li adsorbs on C_3N/C_3B heterostructure.

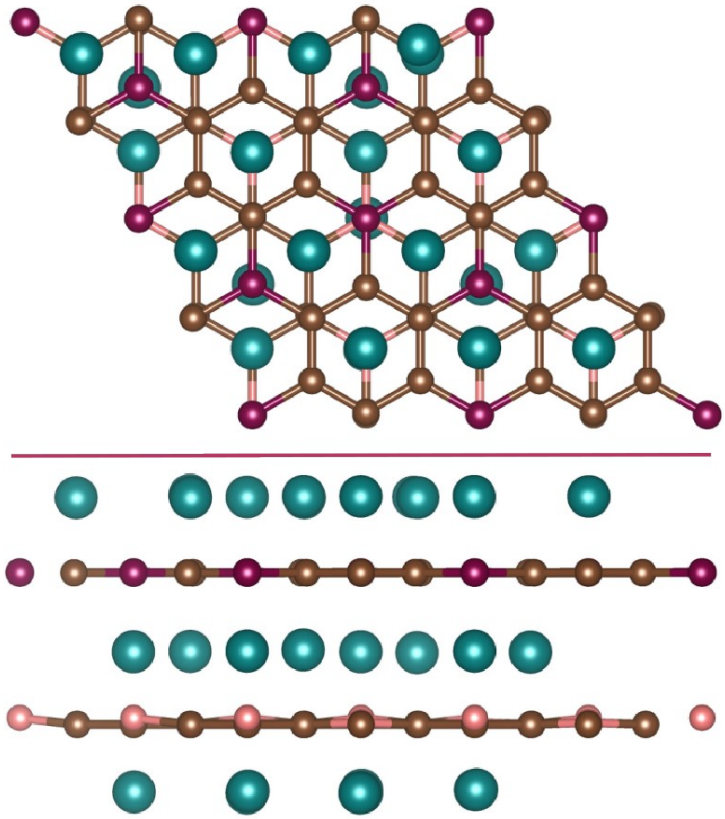

Fig. S4. Top and side views of the maximum possible Li storage in C_3N/C_3B heterostructure.

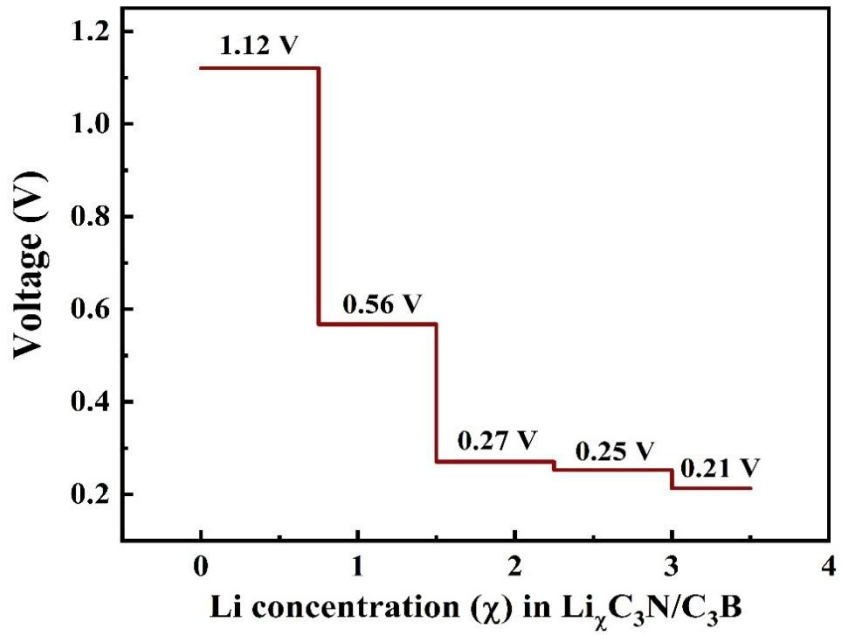

Fig.S5 Calculated voltage that depending on the Li concentration of Li_xC_3N/C_3B systems.

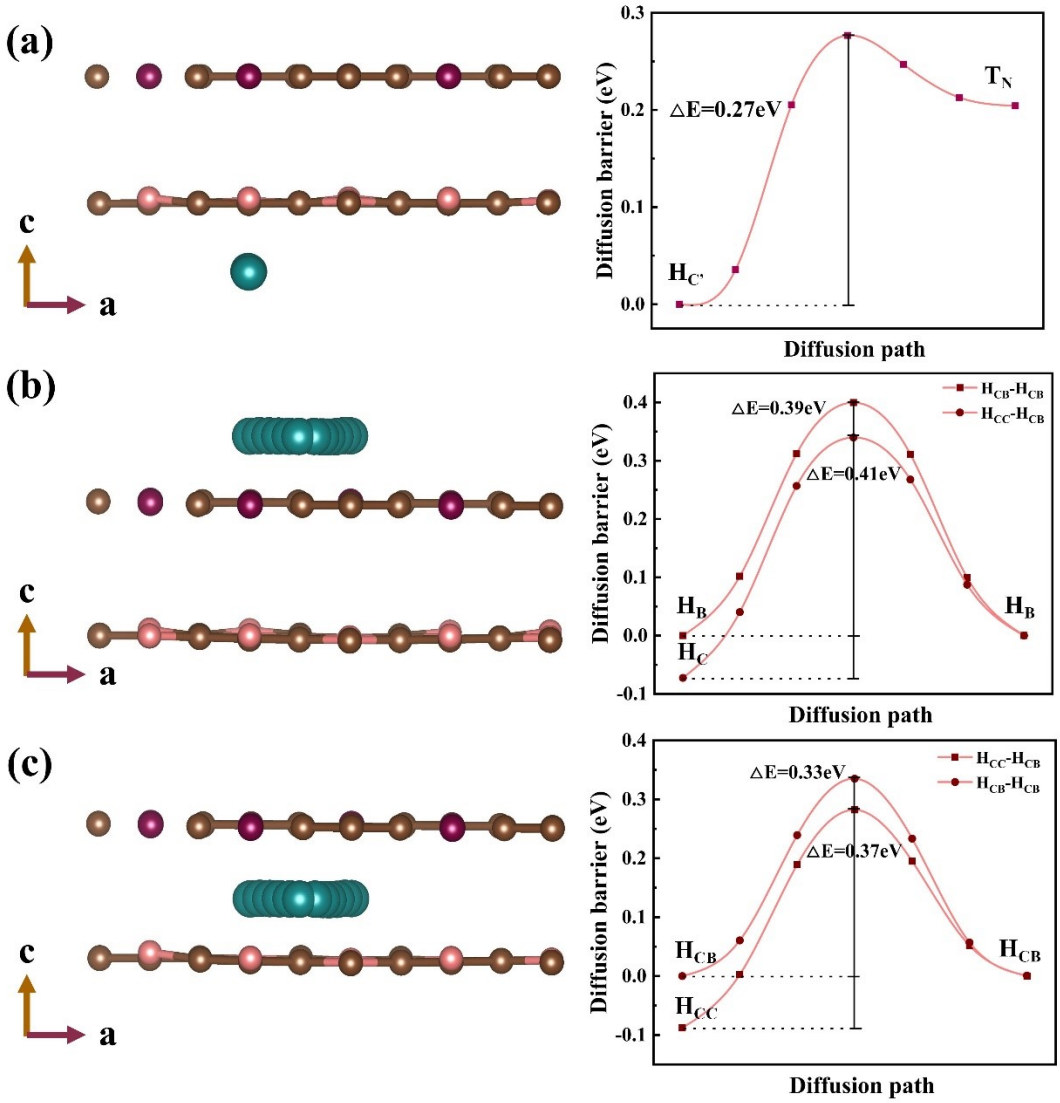

Fig. S6 Front view of migration path and energy barrier of Li diffusion (a) on the outside of C_3N of the C_3N/C_3B heterostructure ($Li/C_3N/C_3B$); (b) on the outside of C_3B of the C_3N/C_3B heterostructure ($C_3N/C_3B/Li$); (c) on the interlayer of C_3N/C_3B heterostructure ($C_3N/Li/C_3B$).

Table S1 The charge value of carbon (Q_C), nitrogen (Q_N), boron (Q_B), and Li (Q_{Li}) atoms at different Li concentrations in C_3N/C_3B heterostructure.

Li concentration (x) in C_3N/C_3B	$Q_{C\ (C3N)}$	$Q_{C\ (C3B)}$	Q_N	Q_B	Q_{Li}
0.00	86.79	112.10	48.77	8.34	0.00
0.75	89.01	114.51	48.73	8.77	0.98

1.50	91.35	115.66	49.06	9.56	2.36
2.25	94.42	116.01	49.15	9.99	4.43
3.00	94.51	119.88	49.04	10.62	5.93
3.50	96.05	117.71	48.75	10.67	10.82