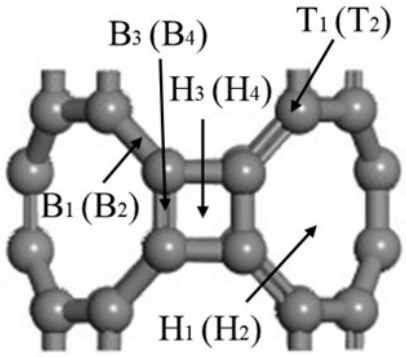

Fig. S1 Structure of T-graphene nanotubes

Table S1 Adsorption energy of lithium ions at different sites inside and outside T-graphene nanotubes

	H_1	H_2	H_3	H_4	T_1
E_{ad} (eV)	-0.51	-0.38	-0.44	-0.30	-0.38
	T_2	B_1	B_2	B_3	B_4
E_{ad} (eV)	-0.36	-0.22	-0.24	-0.31	-0.32

Table S2 Formation energies (E_f) of T-graphene nanotubes with different tube diameters

Tube diameters	(4,0)	(5,0)	(6,0)	(7,0)	(8,0)
E_f (eV)	-6.89	-6.96	-6.99	-7.01	-7.02

Table S3 The B-C bond length of T-graphene nanotubes with tube length N=1, 2, 3 and 4

Bond length	N=1	N=2	N=3	N=4
B-C1 (Å)	1.523	1.527	1.521	1.528
B-C2 (Å)	1.495	1.501	1.507	1.495

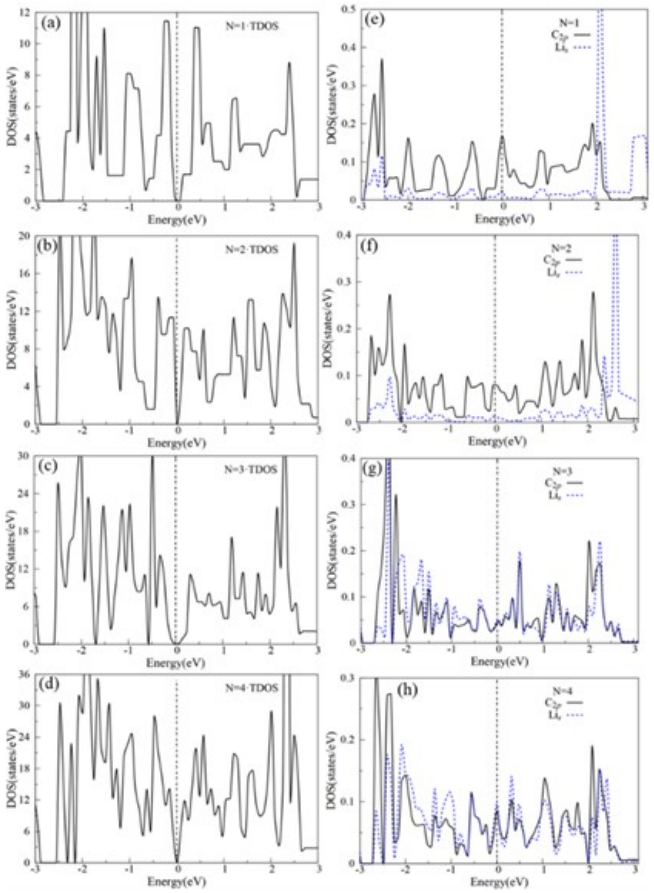

Fig. S2 (a-d) TDOS of intrinsic T-CNTs with different lengths, (e-h) PDOS of T-CNTs with different lengths after adsorbing lithium ions.

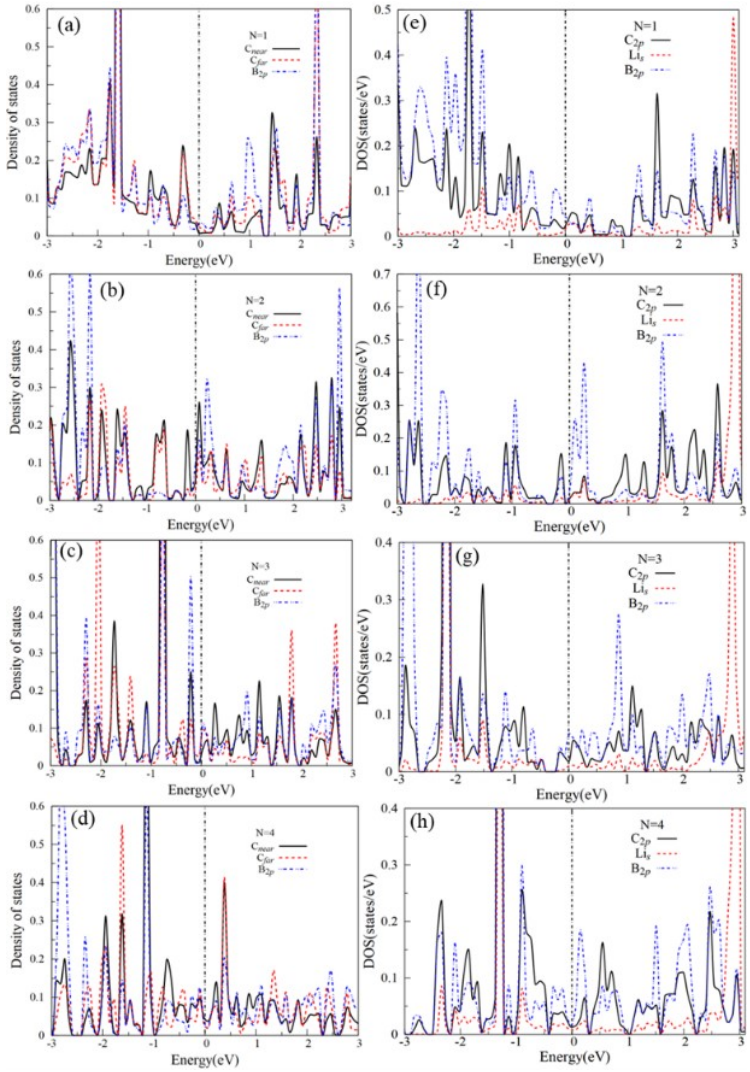

Fig. S3 (a-d) PDOS for B doped T-CNTs of different tube lengths (N=1, 2, 3, 4), (e-h) PDOS of B doped T-CNTs with different tube lengths adsorbing lithium ions.

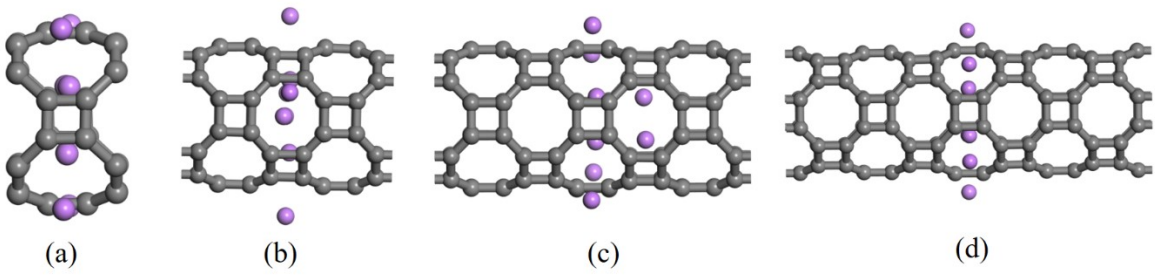

Fig. S4 The adsorption of lithium ions on T-CNTs with tube lengths N=1, 2, 3, and 4. Gray and purple atoms represent C and Li atoms, respectively.

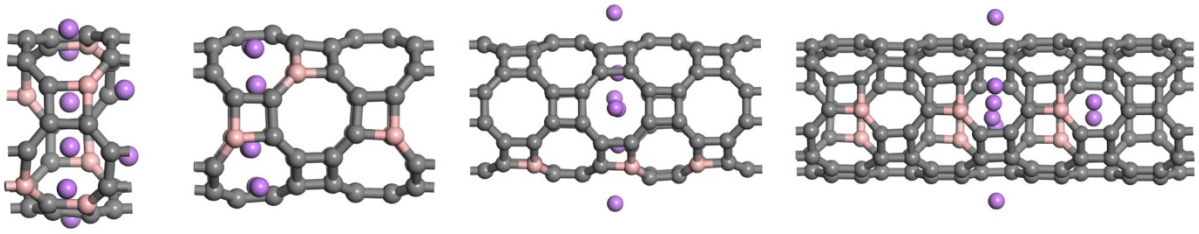

Fig. S5 The adsorption of lithium ions on B doped T-CNTs with tube lengths N=1, 2, 3, and 4. Gray, pink and purple atoms represent C, B and Li atoms, respectively.