

Supporting Information

Two-dimensional Dirac semimetal OD-BC₃ as an ultrahigh-performance anode for Li-, Na-, and K-ion batteries

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Figure S1

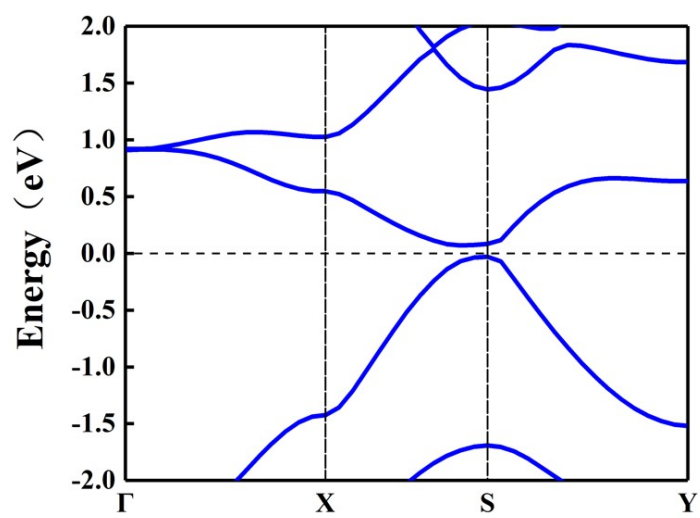


FIG. S1. Electronic band structures of BC₃ calculated using HSE06 functional.

Figure S2

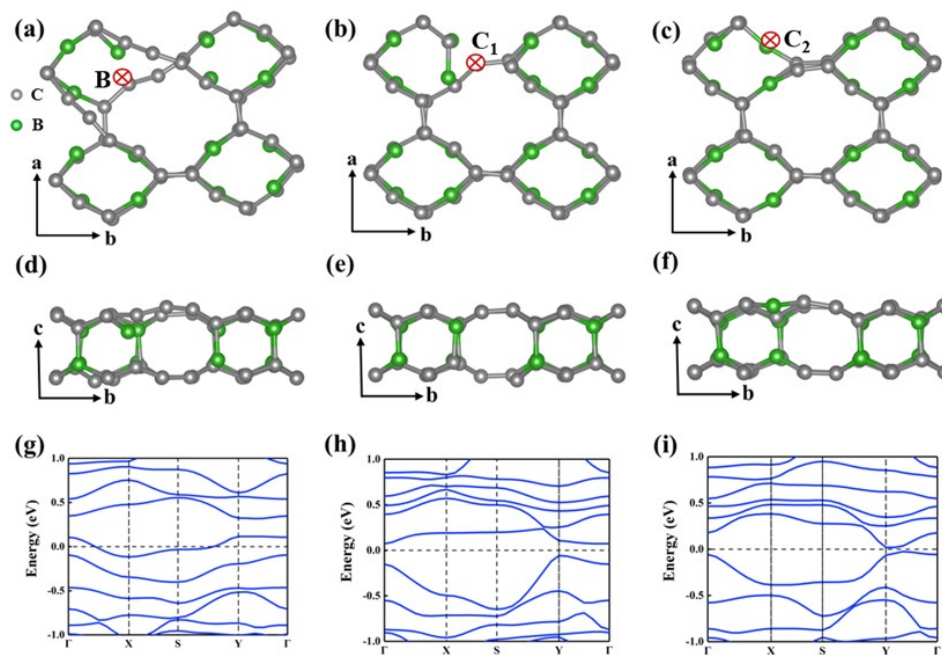


FIG. S2. The atomic structures (top and side views) and corresponding band structures of three vacancy defects in a $2 \times 2 \times 1$ BC_3 supercell are presented: (a-c) boron vacancy (VB), (d-f) carbon vacancy adjacent to boron (VC_1), and (g-i) carbon vacancy distant from boron (VC_2). The defect atoms are highlighted in red for clear visualization.

Figure S3

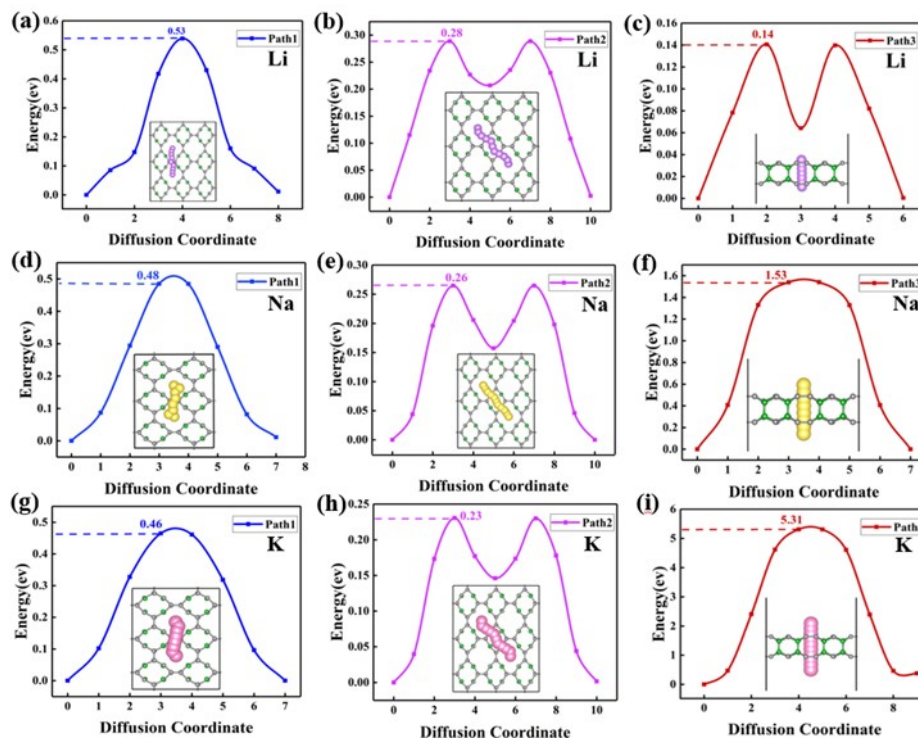


FIG. S3. Diffusion pathways and energy barriers for Li/Na/K migration on BC₃.

Figure S4

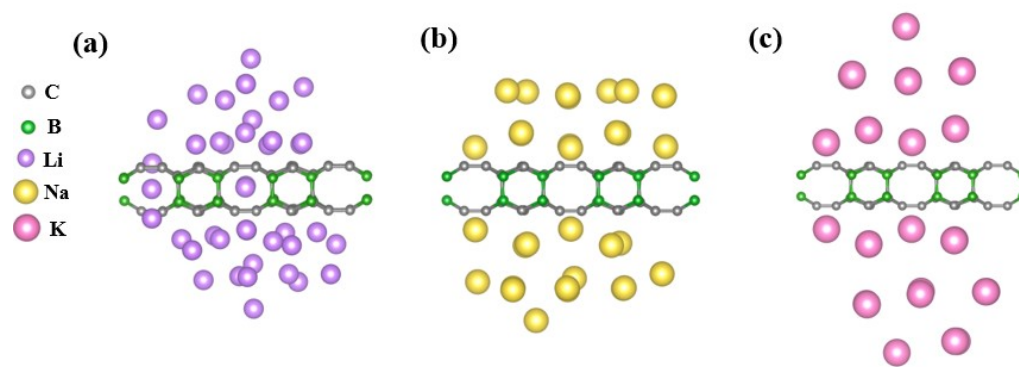


FIG. S4. Optimized maximum reversible adsorption configurations of Li, Na, and K on a $2 \times 2 \times 1$ OD-BC₃ supercell with double-side adsorption (40 Li, 33 Na, and 32 K atoms, respectively).

Figure S5

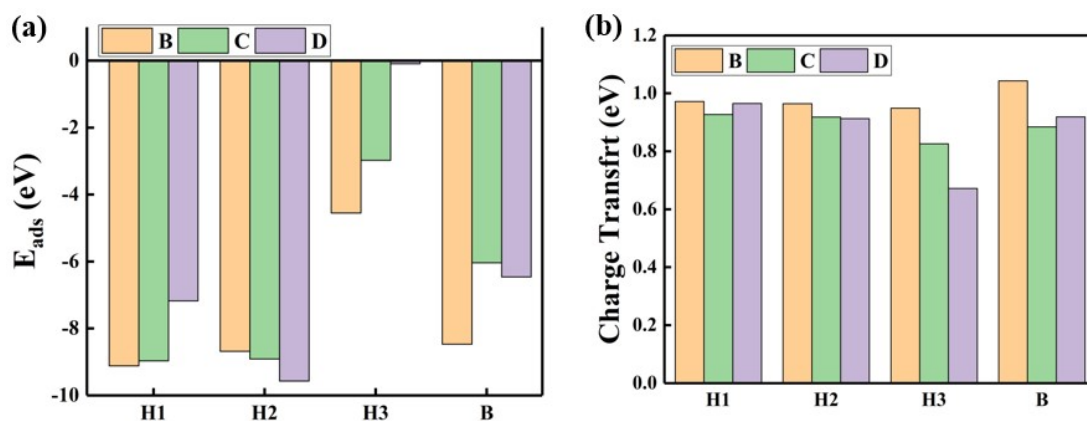


FIG.S5. Adsorption energies (a) and Bader charge transfer (b) for Li, Na, and K at four sites on OD-BC₃, calculated with the optB88-vdW functional.

Table S1. The formation energies of the three defect types.

Ads sites	B	C1	C2
E_{ads}^{defect} (eV)	-4.00	-3.74	-3.83

Table S2. The adsorption energies of solvent molecules (DEC, DMC, EC, and PC) on the BC₃ anode.

Solvent molecule	DEC	DMC	EC	PC
E_{ad} (eV)	-4.00	-3.74	-3.83	-3.91