Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Richly electron-deficient BC_xO_{3-x} anodes with enhanced reaction kinetics for sodium/potassium-ion batteries

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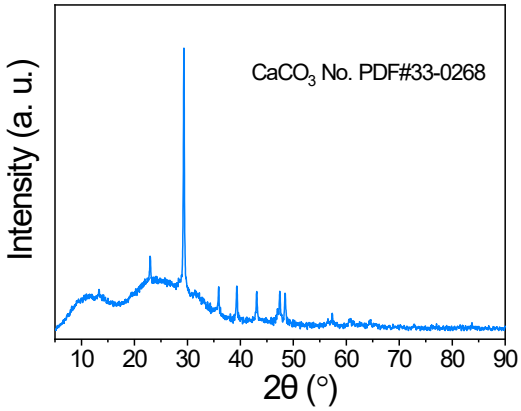

Figure S1 XRD pattern of the PTA@$CaCO_3$ precursor after hydrothermal treatment.

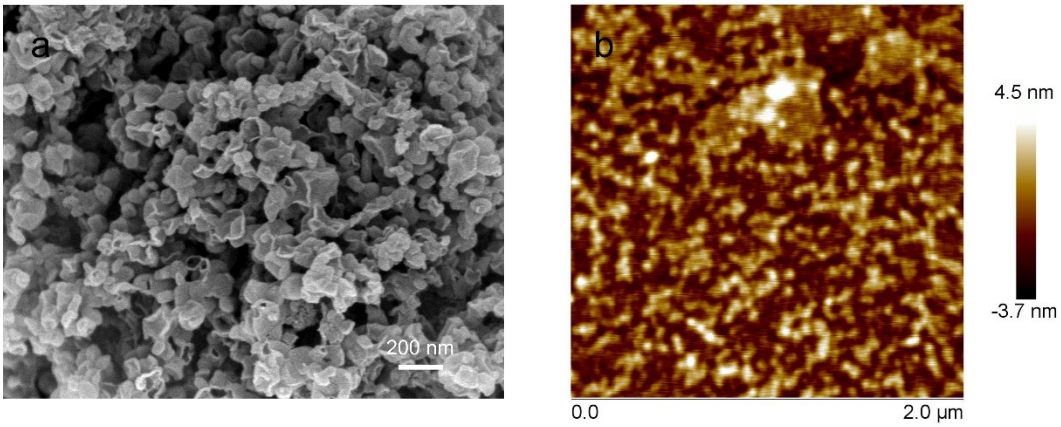

Figure S2 (a) SEM image and (b) AFM image of the BCNCs.

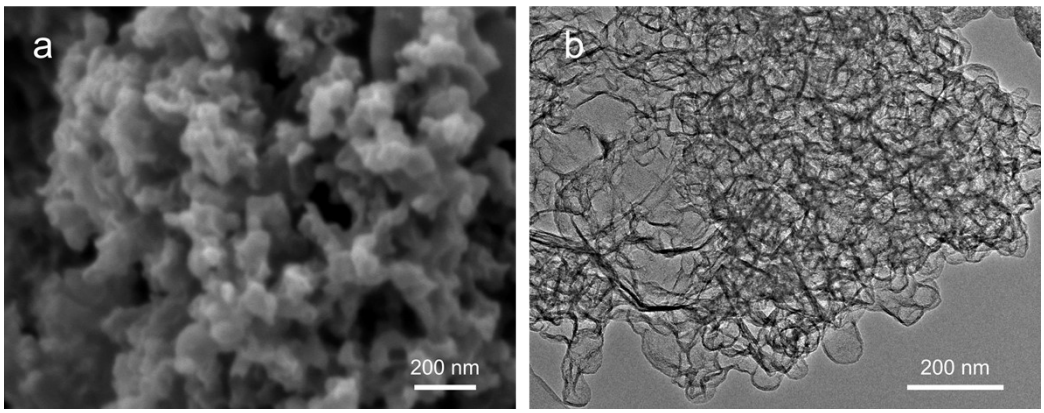

Figure S3 (a) SEM image and (b) TEM image of the pristine CNCs.

Table S1 Components (at. %) of various element species for both BCNCs and CNCs.

No.	B 1s	C1s	O1s
BCNCs	7.29	82.78	9.93
CNCs	0	89.29	10.71

Table S2 Ratios of five types of B 1s components for BCNCs and cycled BCNCs anode in SIBs/PIBs.

No.	B—O		BCO_2		BC_2O		BC_3		B—B	
	BE (eV)	Area (%)	BE (eV)	Area (%)	BE (eV)	Area (%)	BE (eV)	Area (%)	BE (eV)	Area (%)
BCNCs	194.5	7.15	192.9	43.68	192.1	34.07	189.2	5.99	187.3	9.11
Cycled BCNCs anode in SIBs	195.2	34.97	194.4	54.39	192.2	10.64	-	-	-	-
Cycled BCNCs anode in PIBs	195.5	38.96	194.6	48.19	193.3	12.84	-	-	-	-

Table S3 Ratios of five types of C 1s components for BCNCs and cycled BCNCs anode in SIBs/PIBs.

No.	C—C		C—O		C═O	
	BE (eV)	Area (%)	BE (eV)	Area (%)	BE (eV)	Area (%)
BCNCs	284.8	48.65	285.9	25.09	290.0	26.26
Cycled BCNCs anode in SIBs	284.8	51.34	286.3	24.39	288.8	24.28
Cycled BCNCs anode in PIBs	284.7	47.99	285.9	33.76	288.0	18.24

Table S4 Ratios of five types of O 1s components for BCNCs and cycled BCNCs anode in SIBs/PIBs.

No.	O=C		O–C		O–B	
	BE (eV)	Area (%)	BE (eV)	Area (%)	BE (eV)	Area (%)
BCNCs	532.1	59.69	533.3	33.21	537.5	7.10
Cycled BCNCs anode in SIBs	531.5	49.10	532.7	40.95	536.6	9.95
Cycled BCNCs anode in PIBs	531.2	58.50	532.8	41.50	-	-

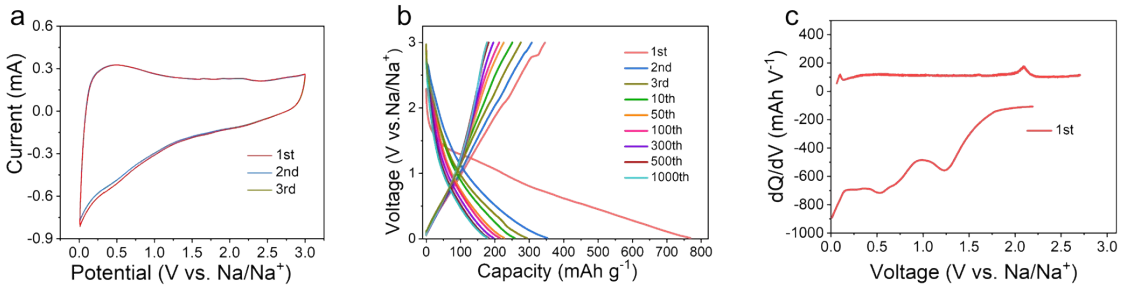

Figure S4 (a) CV curves at 0.1 mV s^{-1} of BCNCs electrode. (b) Discharge-charge curves of BCNCs electrodes at 0.1 A g^{-1}. (c) Corresponding dQ/dV profiles of the initial cycle for BCNCs anode of SIBs.

Table S5 Kinetic parameters calculated by fitting an equivalent circuit of three electrodes.

Samples	Conductivity [a] (× 10^3 S cm^{-1})	SIBs			PIBs		
		R_s (Ω)	R_{ct} (Ω)	σ [b]	R_s (Ω)	R_{ct} (Ω)	σ [b]
CNCs	2.6	7.0	212.6	161.1	0.79	15.06	29.7
BCNCs	9.2	4.5	181.9	160.1	1.06	8.08	18.2
CNCs (after 1000 cycles)	-	3.1	177.2	156.6			
BCNCs (after 1000 cycles)	-	4.2	172.2	150.1	-	-	-

[a] The data were calculated by using 4-point probe method.

[b] The slope of the corresponding lines shown in Figure 3e and S6.

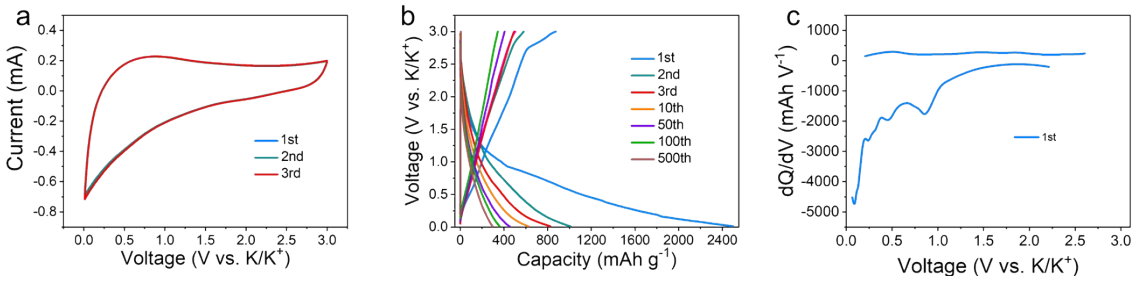

Figure S5 (a) CV curves at 0.1 mV s^{-1} (0.01−3.0 V) of BCNCs electrode. (b) Discharge-charge curves of BCNCs electrodes at 0.1 A g^{-1}. (c) Corresponding dQ/dV profiles of the initial cycle for BCNCs anode of SIBs.

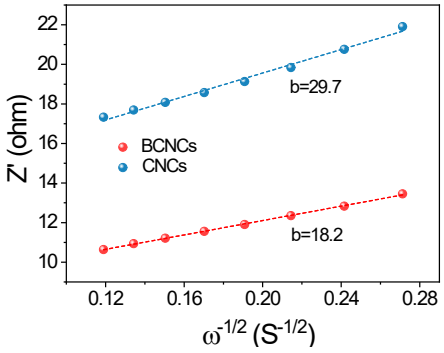

Figure S6 The relationship between Z´ and $\omega^{-1/2}$ of CNCs and BCNCs.

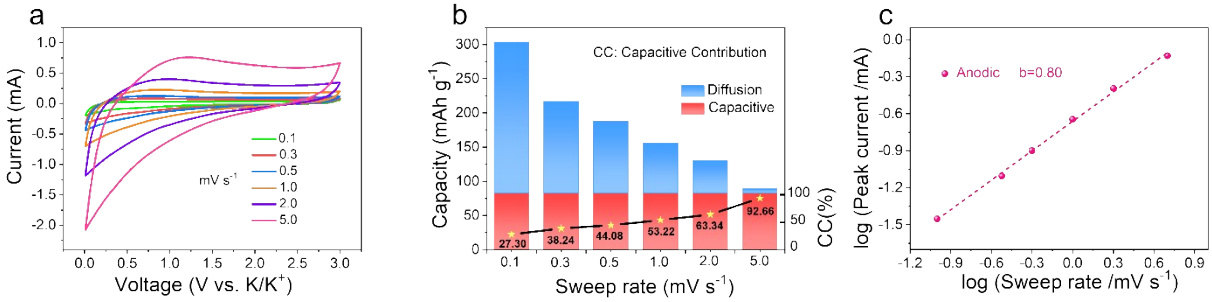

Figure S7 Kinetic analyses for PIBs. (a) CV curves and (b) capacitive contribution under scan rates of 0.1, 0.3, 0.5, 1.0, 2.0 and 5.0 mV s^{-1} and (c) The *b* values plotted for the potential anodic and cathodic peak of BCNCs electrodes.

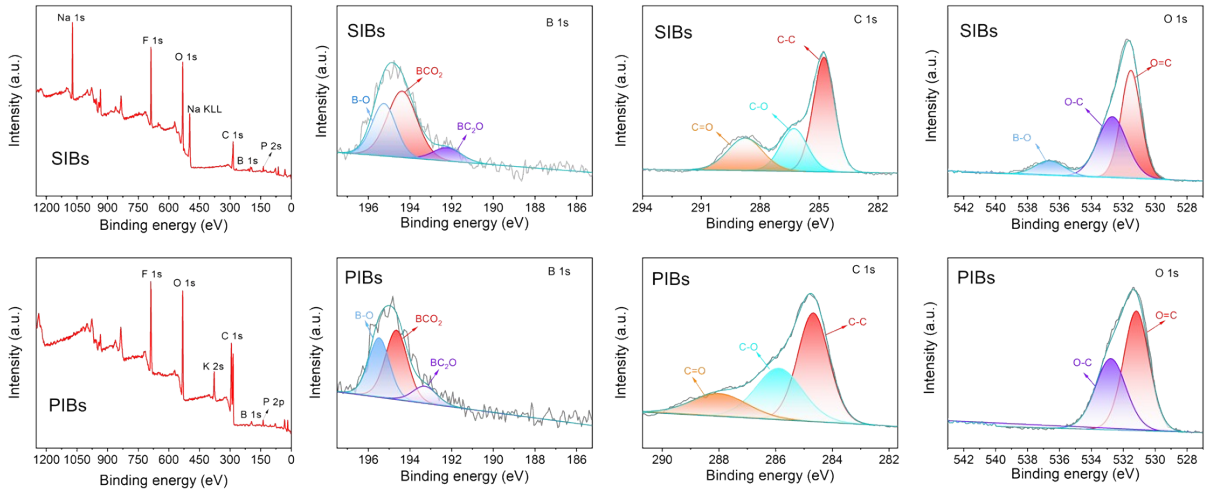

Figure S8 XPS survey spectra and the high-resolution XPS spectra of the cycled BCNCs anode in SIBs and PIBs.

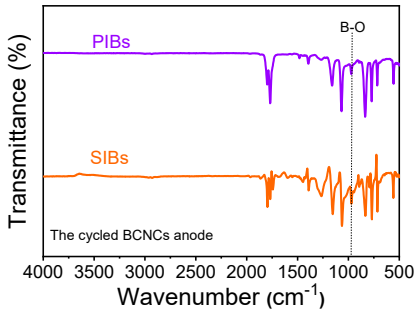

Figure S9 FT-IR spectra of the cycled BCNCs anode in SIBs and PIBs.

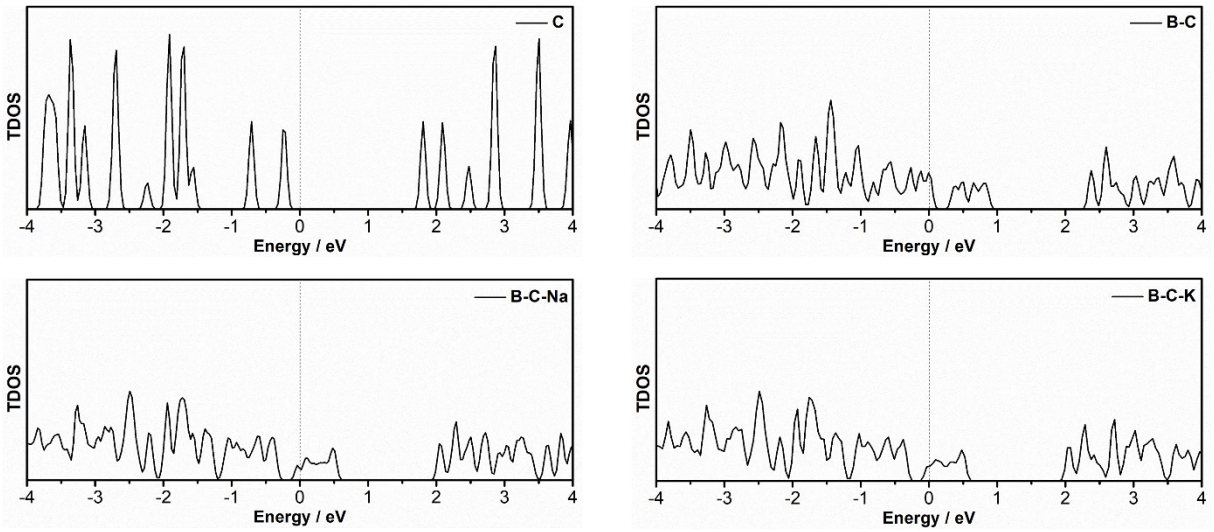

Figure S10 Total density of states (TDOS) for (a) C; (c) B doped C; (e) Na/B doped C; (g) K/B doped C.

Table S6 The comparison analysis of the carbon-based anodes for SIBs.

Material/electrode	Cycling/rate performance (mAh g^{-1})	Year [References]
Carbon-coated NiO/Ni composites (C-NiO/Ni)	83 at 0.1 A g^{-1} after 150 cycles	2021 [1]
TiO_2 carbon nanofiber composite (TiO_2/CNF)	193 at 0.1 A g^{-1} after 100 cycles	2021 [2]
Na_2CrO_4/C nanocomposite (NCrO/C)	166 at 0.1 C after 100 cycles	2021 [3]
Carbon flakes (CF)	131 at 0.1 A g^{-1} after 100 cycles	2021 [4]
$NaFe(MoO_4)_2$ microstructure (NFMO)	100 at 0.1 A g^{-1} after 500 cycles	2021 [5]
Sulfur-doped carbon (SDC)	118 at 50 mA g^{-1} after 100 cycles	2021 [6]
Hollow carbon microbox (HCMB)	140 at 0.5 A g^{-1} after 500 cycles	2020 [7]
Nitrogen-doped porous carbon (NDPC)	202 at 0.5 C after 100 cycles	2020 [8]
N-doped carbon hollow spheres (NDCHS)	260 at 84 mA g^{-1} after 300 cycles	2019 [9]
Hard carbon spheres (HCS)	181 at 0.1 A g^{-1} after 500 cycles	2020 [10]
Hollow porous carbon spheres (HPCS)	104 at 0.5 A g^{-1} after 10 cycles	2021 [11]
hollow BC_xO_{3-x} nanocages (BCNCs)	176 at 0.1 A g^{-1} after 1000 cycles	This work

Table S7 The comparison analysis of the carbon-based anodes for PIBs.

Material/electrode	Cycling/rate performance (mAh g^{-1})	Year [References]
Nitrogen-doped carbon microspheres (NCMSs)	95 at 0.5 A g^{-1} after 400 cycles	2021 [12]
Carbon nanofibers (CNFs)	214 at 100 mA g^{-1} after 5 cycles	2018 [13]
Microcrystalline graphite carbon (GC)	172 at 0.1 A g^{-1} after 200 cycles	2021 [14]
Carbon supported tin sulfide (SbS/C)	76 at 0.2 A g^{-1} after 200 cycles	2021 [15]
Nitrogen-doped carbon nanosheet (NCNS)	253 at 50 mA g^{-1} after 200 cycles	2021 [16]
Porous nanoflake (PNF)	200 at 0.1 C after 20 cycles	2020 [17]
N-doped porous carbon (NDPC)	256 at 50 mA g^{-1} after 10 cycles	2020 [18]
Hard carbon (HC)	232 at 0.1 C after 100 cycles	2019 [19]
3D hierarchically porous carbon (3D-PC)	276 at 50 mA g^{-1} after 100 cycles	2018 [20]
Activated carbon (AC)	209 at 0.1 A g^{-1} after 10 cycles	2017 [21]
CNT-modified graphited carbon (CNT-GC)	56 at 2 A g^{-1} after 10 cycles	2019 [22]
hollow BC_xO_{3-x} nanocages (BCNCs)	133 at 0.1 A g^{-1} after 500 cycles	This work

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