

Electronic Supplementary Information

Computational Details

All density functional theory (DFT) calculations were performed using the Vienna ab initio simulation package (VASP). Generalized gradient approximation (GGA) in the form of Perdew–Burke–Ernzerhof (PBE) functional was employed for the electron exchange and correlation energy. For Kohn–Sham wave functions, the cutoff energy of corresponding plane-wave basis set was set to 450 eV. The K points meshing was obtained from the Monkhorst-Pack scheme. The atomic coordinates are fully relaxed using the conjugate gradient method. The energy convergence criterion for the electronic self-consistent iteration and the force for atomic relaxation were set to 10^{-4} eV and 0.02 eV/Å, respectively. A vacuum width of 15 Å along the Z axis was created to ensure negligible interaction. The adsorption energies of Sodium ions were calculated according to the equation as follows:

$$\Delta E_{\text{Na}^*} = E_{\text{Na}^*} - (E_{\text{Na}} + E_{\text{slab}})$$

where E_{Na^*} , E_{Na} and E_{slab} are energies of the slab with adsorbed Na, Na and the clean slab, respectively.

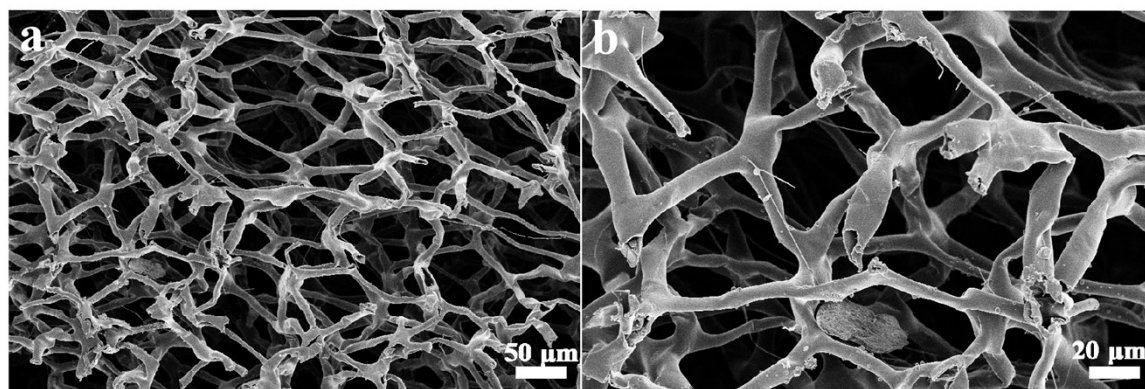


Fig. S1 (a, b) SEM images of the biomass juncus.

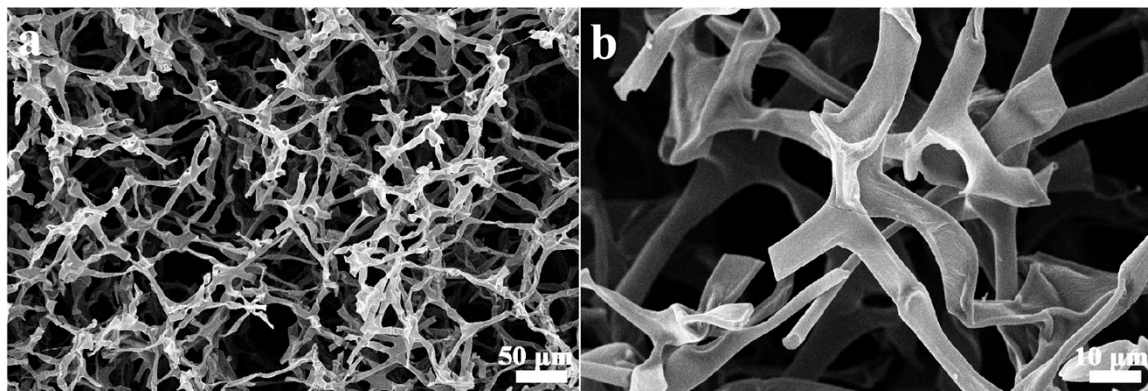


Fig. S2 (a, b) SEM images of the biomass juncus derived three-dimension interconnected carbontube.

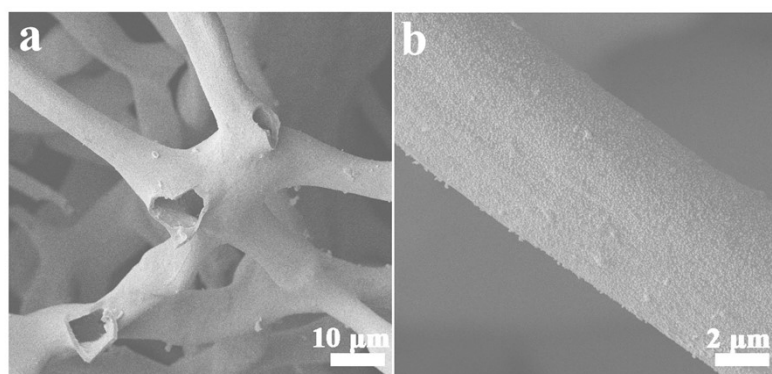


Fig. S3 (a, b) SEM images of the Ni/Co/JDC-based composites.

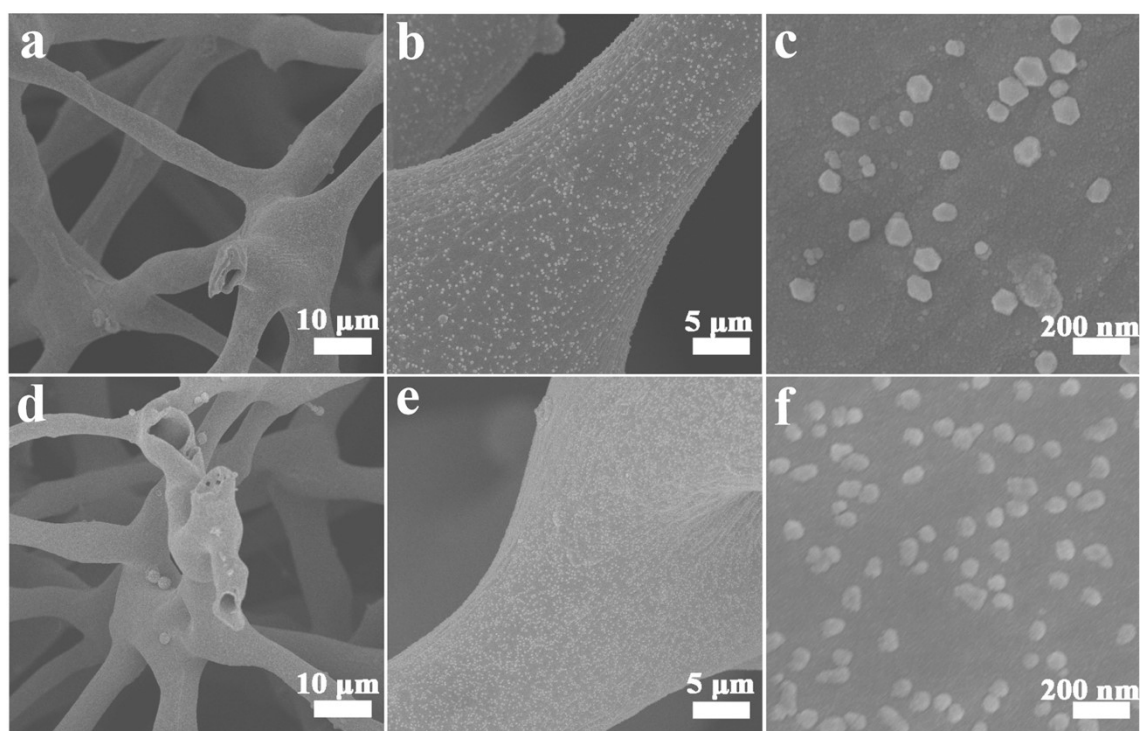


Fig. S4 SEM images of the composites: (a-c) NiS/JDC composites, (d-f) CoS/JDC composites.

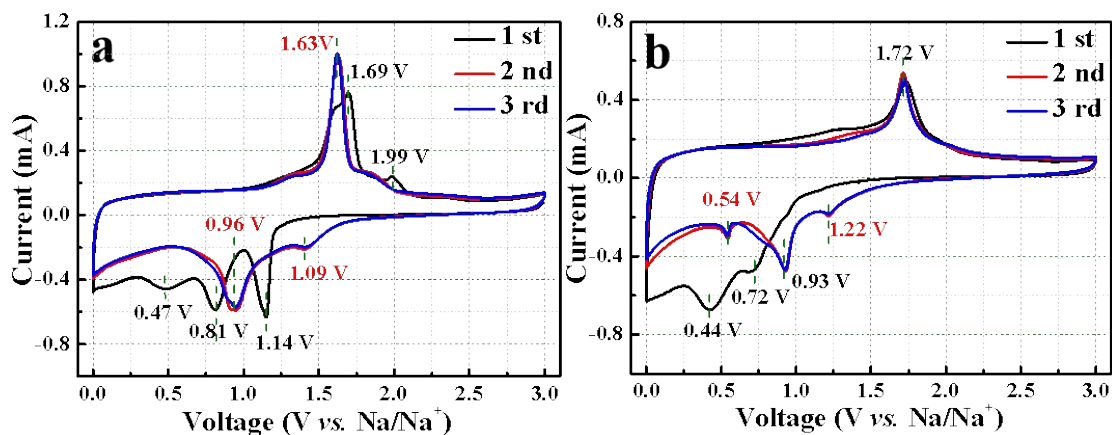


Fig. S5 Initial three CV curves of the electrodes at 0.5 mV s⁻¹: (a) NiS/JDC, (b) CoS/JDC.

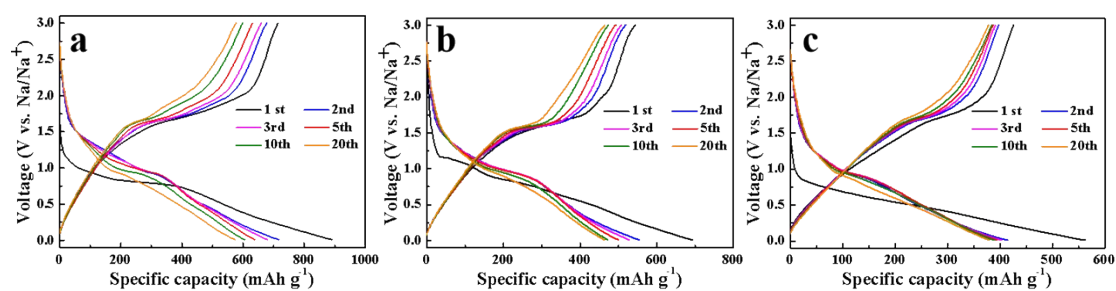


Fig. S6 GCD profiles of the electrodes at 1.0 A g⁻¹: (a) NiCo₂S₄/JDC, (b) NiS/JDC, (c) CoS/JDC.

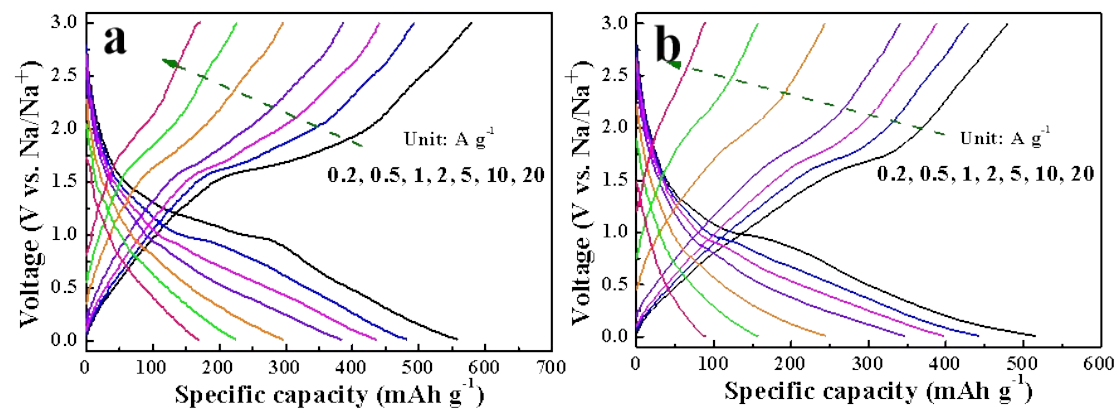


Fig. S7 GCD profiles of the electrodes at different rates: (a) NiS/JDC, (b) CoS/JDC.

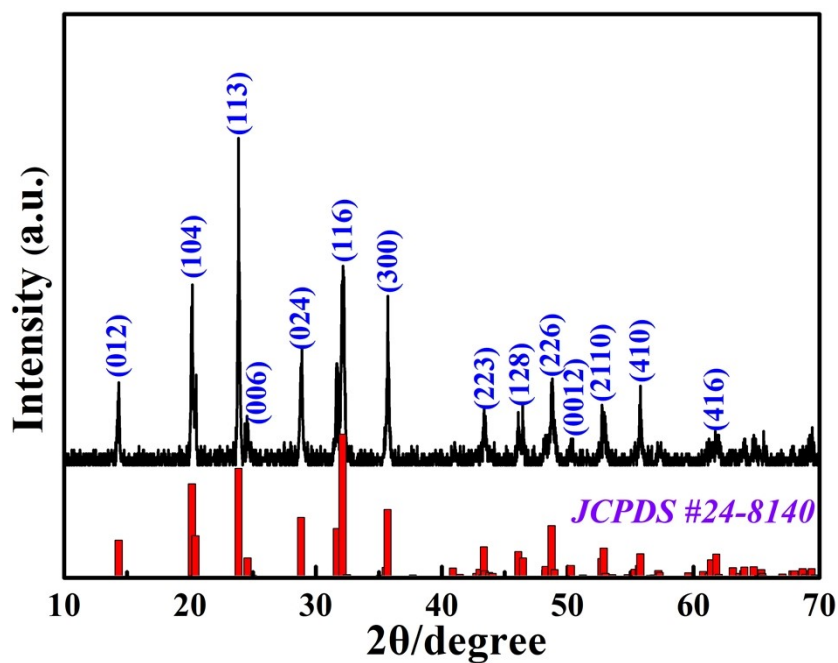


Fig. S8 XRD pattern of the $\text{Na}_3\text{V}_2(\text{PO}_4)_3@\text{C}$.

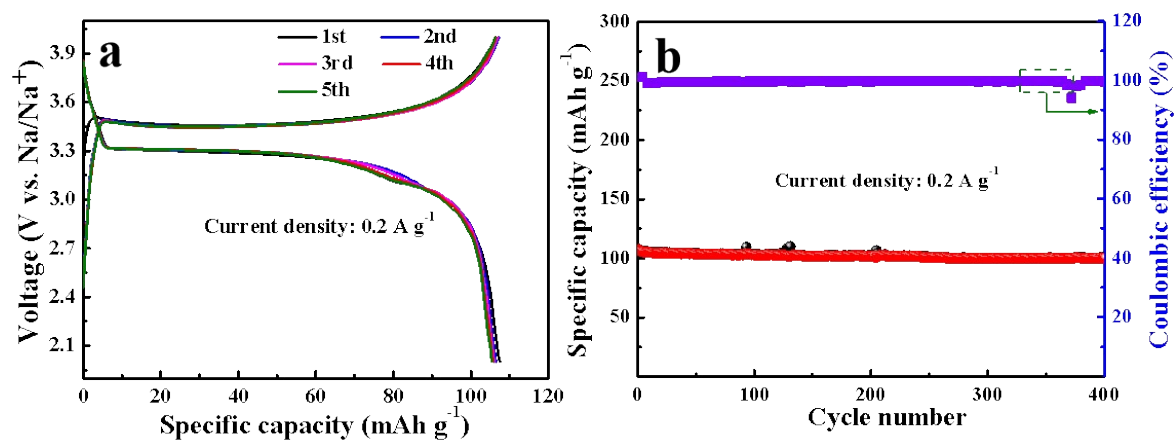


Fig. S9 GCD profiles (a) and cycling performance (b) of the $\text{Na}_3\text{V}_2(\text{PO}_4)_3@\text{C}$ at 0.2 A g^{-1} .

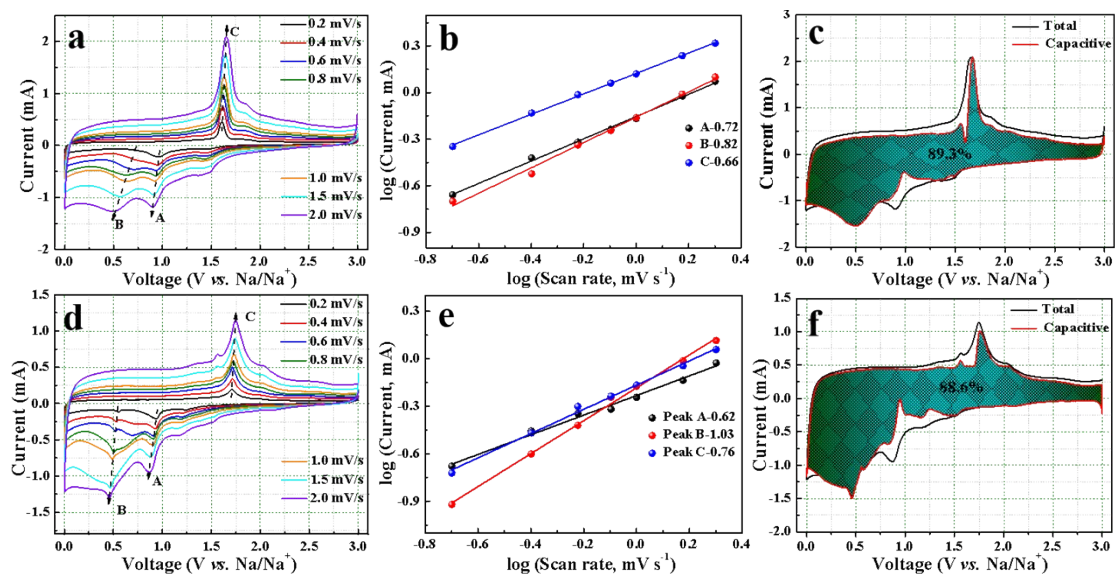


Fig. S10 CV curves at different scanning speeds, b values at three redox peaks, and pseudocapacitive contribution at 2.0 mV s⁻¹ of the electrodes: (a, b, c) NiS/JDC, (d, e, f) CoS/JDC.

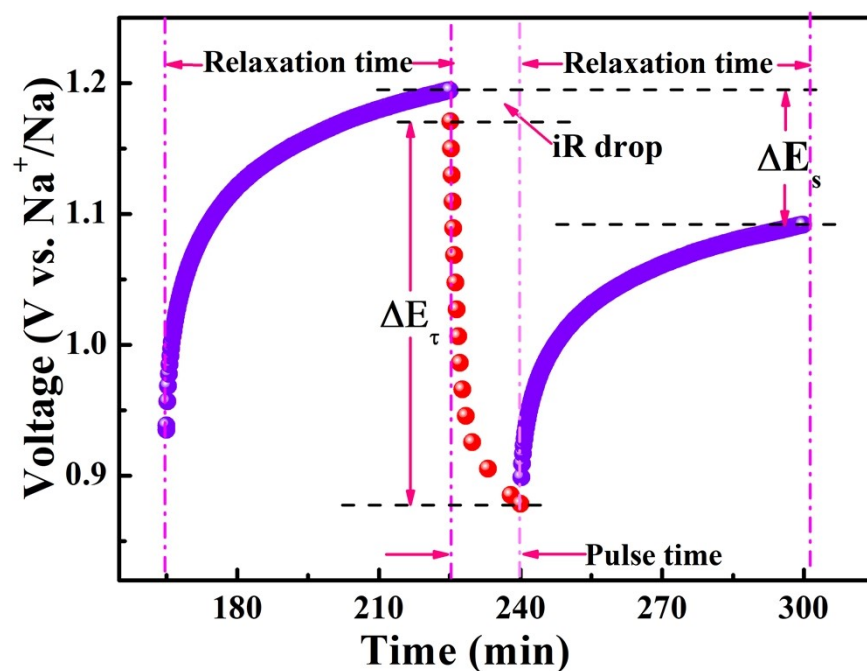


Fig. S11 The detailed voltage response during a single current pulse.

In GITT measurement, the cell was charged and discharged at 0.2 A·g⁻¹ for 10 min followed by an open-circuit stand for 60 min until a steady state was achieved to the voltage range 0.01–3.0 V. The sodium diffusion coefficient (D_{Na^+}) can be figured out using the simplified Fick's second law:

$$D = \frac{4L^2}{\pi\tau} \left(\frac{\Delta E_s}{\Delta E_\tau} \right)$$

Where L (cm) symbolizes the sodium ion diffusion distance, which can be identified as the thickness of the electrodes for compact electrode. And ΔE_s (V) and ΔE_{τ} (V) refer to the difference in the steady state potential of the step at plateau, and the total change of the voltage during a constant current pulse time excluding the iR drop as depicted in Fig. S11.

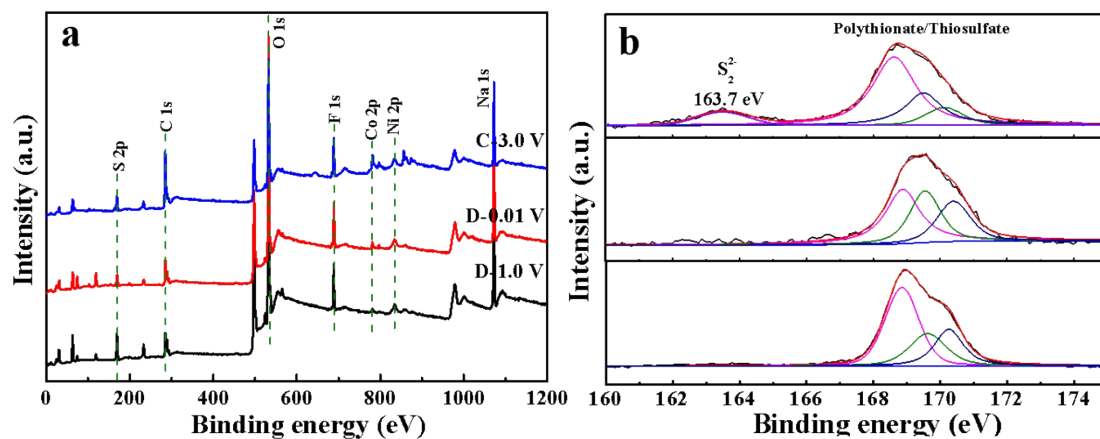


Fig. S12 XPS survey spectra (a) and high-resolution S 2p spectra of the NiCo₂S₄/JDC composites at different discharged and charged states.

Table S1 Comparison of cycle lifespan and specific capacity of the NiCo₂S₄/JDC composites with previous reported NiCo₂S₄- and CoNi₂S₄-based anodes in SIBs systems.

Materials	Voltage window (V)	Rate (A g ⁻¹)	Cycle number	Capacity (mAh g ⁻¹)	Ref.
Flower-like NiCo ₂ S ₄ nanosheets	0.3-3.0	2.0	500	376.0	1
NiCo ₂ S ₄ @rGO	0.01-3.0	0.1	300	387.6	2
NiCo ₂ S ₄ @CNF	0.01-3.0	0.05	80	291.1	3
NiCo ₂ S ₄ @MoS ₂	0.01-3.0	3.2	400	157.8	4
NiCo ₂ S ₄ NW/GF	0.01-3.0	0.5	200	529.0	5
Coral-loke Ni _{1.01} Co _{1.99} S ₄	0.3-2.7	1.0	1000	350.0	6
NiCo ₂ S ₄ @NC	0.4-3.0	6.0	5000	395.6	7
CoNi ₂ S ₄ @rGO	0.01-3.0	0.1	50	430.0	8
CoNi ₂ S ₄ @C	0.01-3.0	0.1	50	438.0	9
NiCo ₂ S ₄ @CNT	0.01-3.0	1.0	7500	454.0	10
NiCo ₂ S ₄ /JDC	0.01-3.0	20.0	3200	231.7	This work

Table S2 Fitting result of EIS spectra in Fig. 4g with the equivalent circuit proposed

Samples	R _s (Ω)	R _{ct} (Ω)
NiCo ₂ S ₄ /JDC	10.37	9.46
NiS/JDC	11.34	10.28
CoS/JDC	12.72	28.17

References

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