Support Information

Experimental Design and Theoretical Calculation for Sulfur-Doped Carbon Nanofibers as High Performance Sodium-Ion Battery Anode

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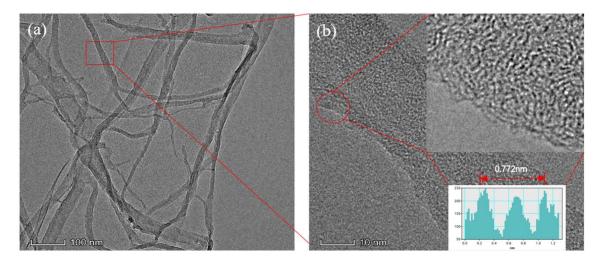


Figure S1. a) The transmission electron microscopy (TEM) of CNFs. b) The inserts are the high-resolution TEM

image and lattice distance of S-CNFs in (a) with red rectangle.

Table S1. The surface analysis reports for CNFs and S-CNFs.

| | Total surface area | Micropore surface area | |
|--------|--------------------|------------------------|--|
| | (m² g-1) | (m² g ⁻¹) | |
| CNFs | 465 | 230 | |
| S-CNFs | 669 | 439 | |

Table S2. The carbon, sulfur and oxygen contents from XPS and element analysis.

| | | Chemical composition (wt%) | | Element content (wt%) |
|--------|---|----------------------------|--------------|--------------------------|
| | | Atomic content | Mass content | |
| S-CNFs | С | 84.34 | 76.31 | 76.31 |
| | О | 11.67 | 14.06 | 13 |
| | S | 7.98 | 15.00 | 17.44 |
| CNFs | С | 89.16 | 85.84 | 90 |
| | О | 10.63 | 13.63 | 14.16 |
| | S | - | - | - |

Table S3. The kinetic parameters obtained from equivalent circuit fitting of experimental data for CNFs, S-CNFs.

| | $R_s(\Omega)$ | R_{ct} (Ω) |
|--------|---------------|-----------------------|
| CNFs | 3.488 | 460.7 |
| S-CNFs | 1.838 | 325.7 |

Noting: Randles equivalent circuit for CNFs, S-CNFs electrode/electrolyte interface. R_s is the electrolyte resistance. CPE₁ and R_{ct} are the capacitance and charge-transfer resistance, respectively. W_1 is the Warburg impedance related to the diffusion of sodium ions into the bulk electrodes.

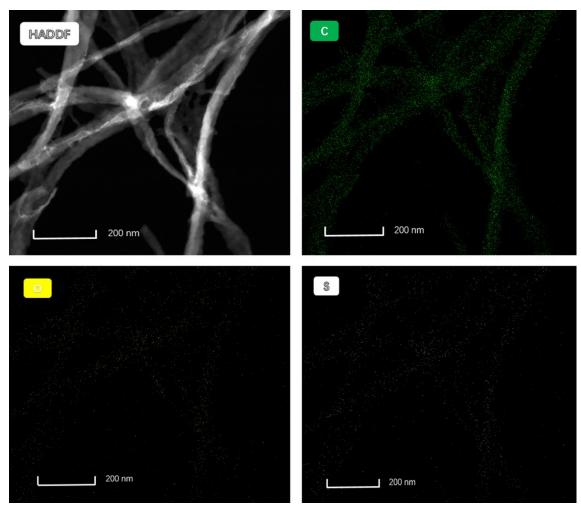


Figure S2. The HADDF (High-Angle Annular Dark Field) image and Mappings of element C, O, S by STEM for S-CNFs.

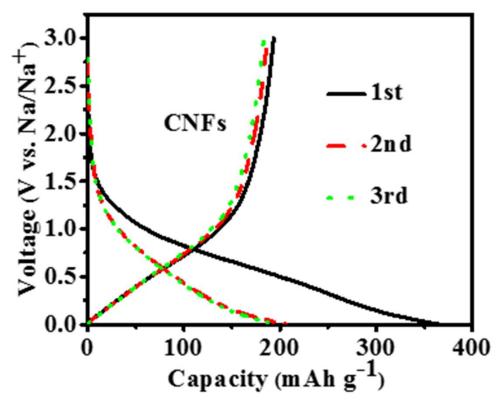


Figure S3. The discharge/charge curves at 50 A $\rm g^{\text{-}1} for\ CNFs.$

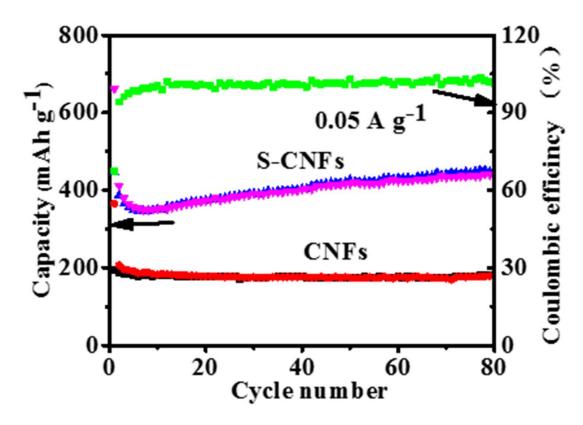


Figure S4. The cycling performances of CNFs and S-CNFs at 0.05 A g^{-1} .

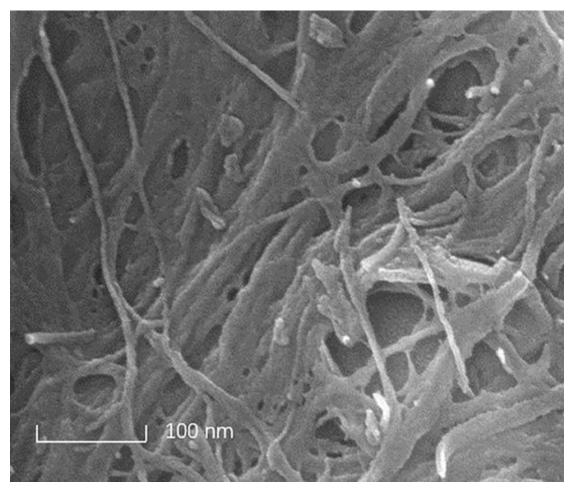
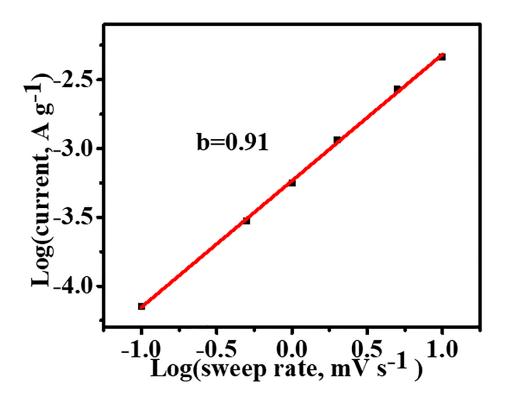


Figure S5. The SEM image of after 1000 cycles for S-CNFs.



 $\textbf{Figure S6.} \ \ \textbf{The b-value calculated by log (sweep rate)-log (peak current) curve at anode peak.}$

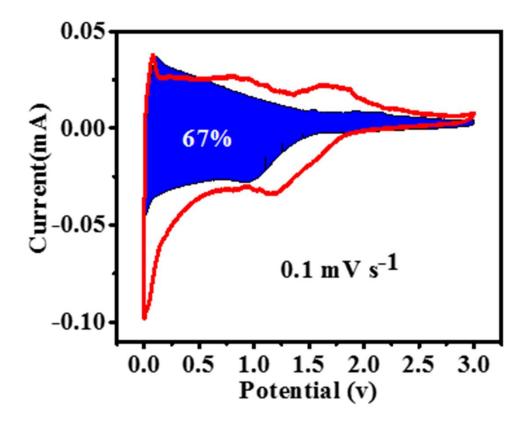


Figure S7. The contribution and distribution of the electrochemical capacitance at 0.1 mV s⁻¹.

Supplementary method. In order to obtain the contributions of capacitance and diffusion, various cyclic voltammetry measurements (CVs) were performed at range of 0.1-10 mV s⁻¹. Firstly, according to the $I(\nu)$ = $a\nu^b$, the controlled process was determined by the b value. Then, the individual capacity was separated by the formula: $I(\nu)$ = $k_1\nu^{1/2}$ + $k_2\nu$. The current values at a fixed voltage were calculated by CVs at sweep rates of 0.1-10 mV s⁻¹. Consequently, the k_1 and k_2 at a fixed voltage were obtained by drawing plots of $I/\nu^{1/2}$ vs. $\nu^{1/2}$. Finally, the k_1 and k_2 at different voltages could be obtained, and the capacitive induced and diffusion induced contributions were determined, respectively.

Table S4. The energy values at different doping sites.

| Doping sites | D_1 | D ₂ | D ₃ | D_4 |
|---------------|------------|----------------|----------------|------------|
| Energy values | 40402.007 | 40403 505 | 40402.002 | 10103.553 |
| (eV) | -10402.087 | -10402.595 | -10402.003 | -10402.663 |