Supplementary Information (SI) for Journal of Materials Chemistry A.

Supplementary Information for

Electrospun Fe-ZIF Derived Carbon Nanofibers for Boosting Adsorption and Redox Kinetics of Polysulfides in Lithium Sulfur Batteries

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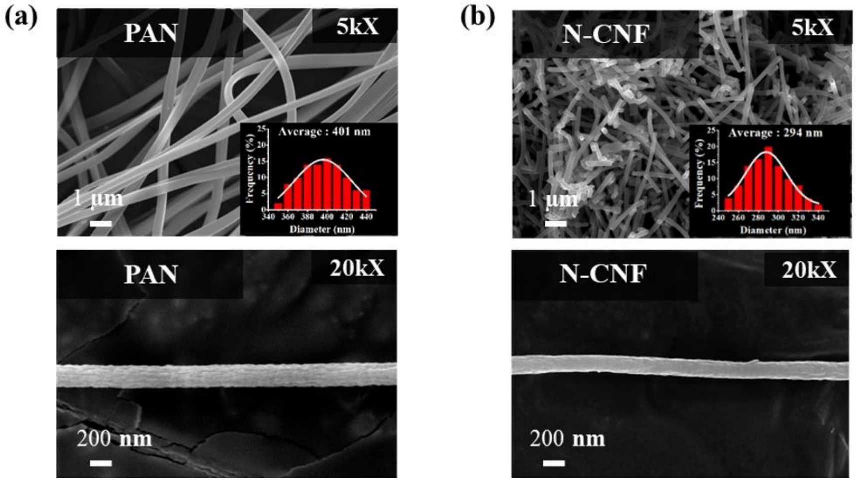

Fig. S1 SEM images and size distributions of (a) PAN fiber and (b) N-CNF.

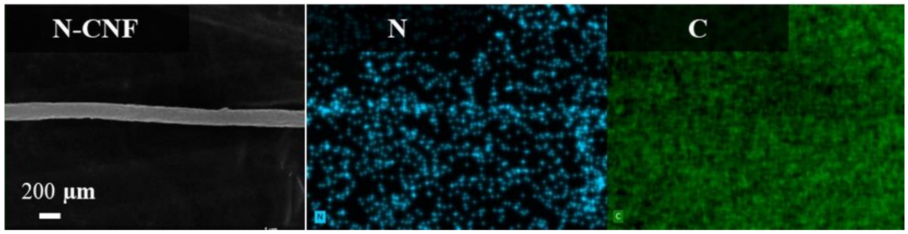

Fig. S2 EDS mapping images of N-CNF.

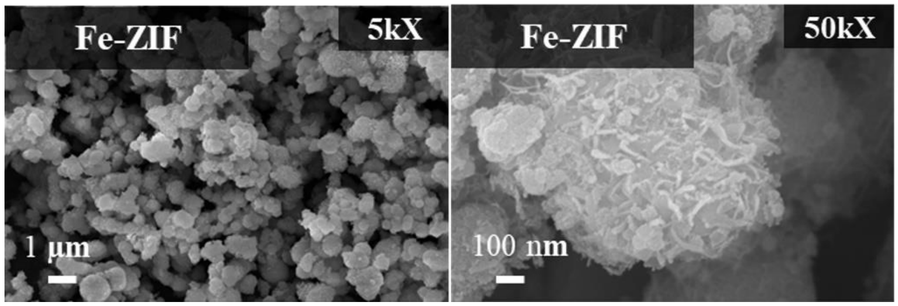

Fig. S3 SEM images of Fe-ZIF particles.

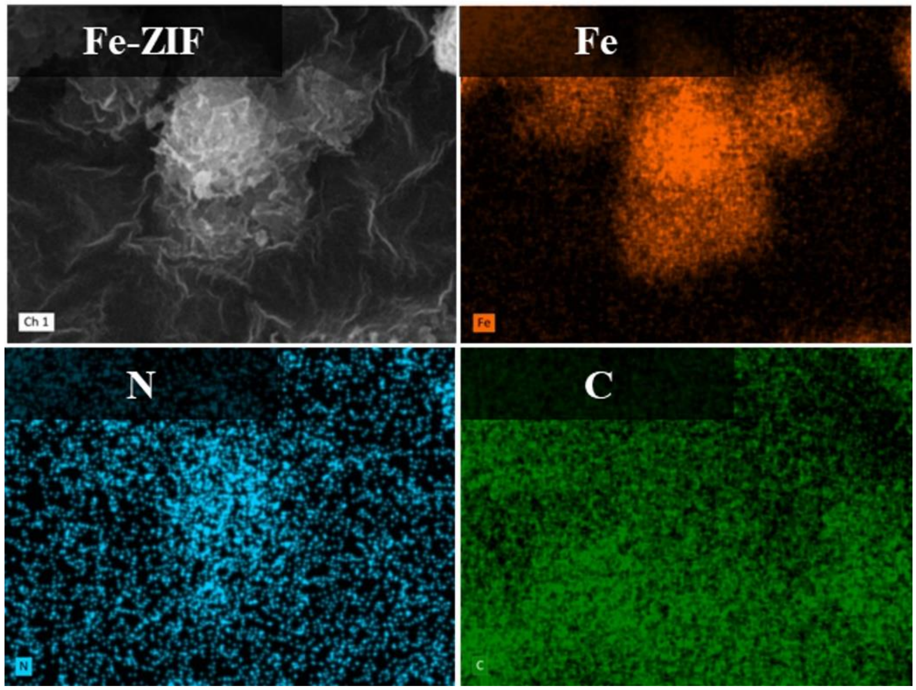

Fig. S4 EDS mapping images of Fe-ZIF particles.

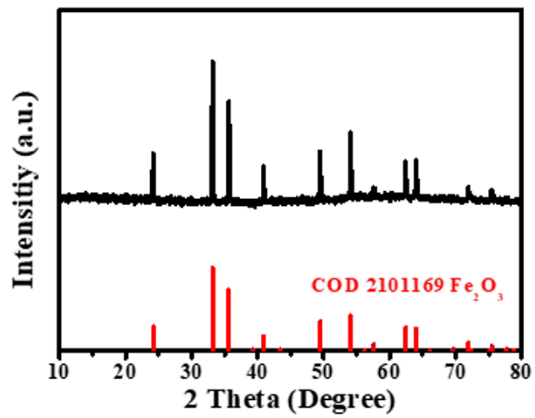

Fig. S5 XRD pattern of the residue of Fe/N-CNF after TGA analysis.

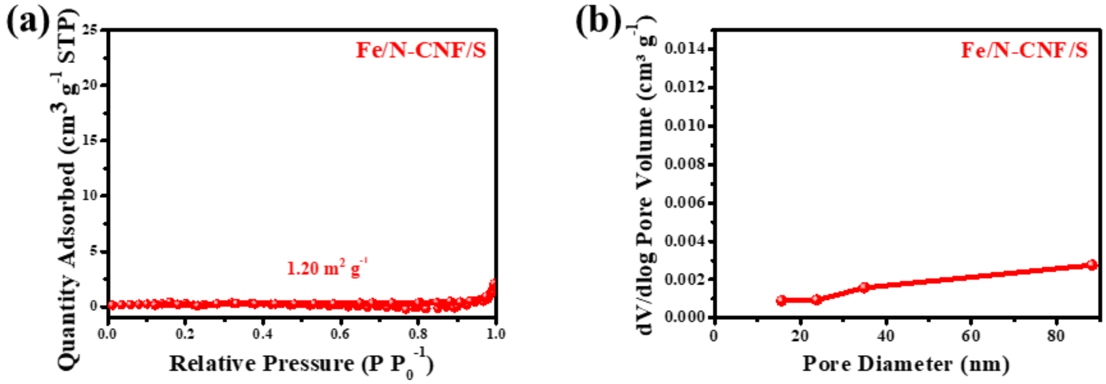

Fig. S6 (a) CV profiles and (b) Nyquist plots of the cells with Fe/N-CNF, N-CNF, and sulfur as the cathodes after 30 cycles.

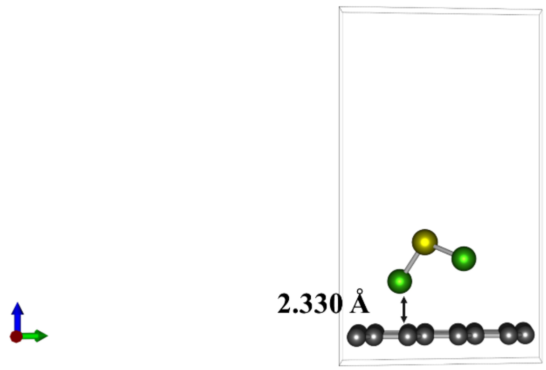

Figure S7. Modeling of the structure after the adsorption of Li_2S on graphene.

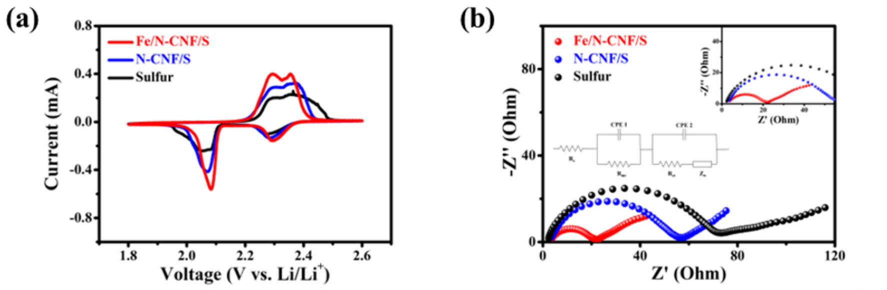

Fig. S8 (a) CV profiles and (b) Nyquist plots of the cells with Fe/N-CNF, N-CNF, and sulfur as the cathodes after 30 cycles.

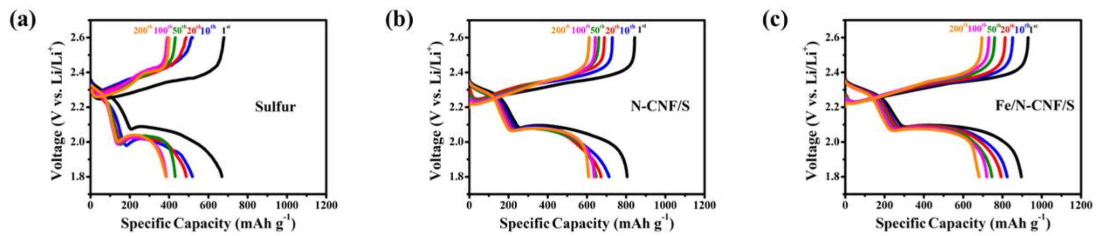

Fig. S9 Galvanostatic charge and discharge curves of the cells with (a) sulfur, (b) N-CNF and (c) Fe/N-CNF as the cathodes measured at 0.2 C for 1st, 10th, 50th, 100th, and 200th cycles.

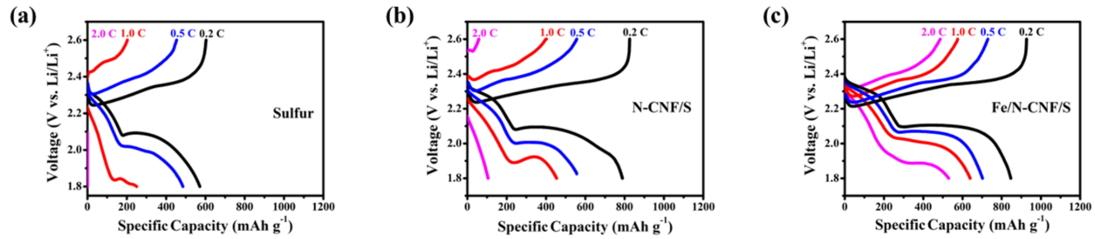

Fig. S10 Galvanostatic charge and discharge curves of the cells with (a) sulfur, (b) N-CNF and (c) Fe/N-CNF as the cathodes measured at different rates 0.2 to 2.0 C.

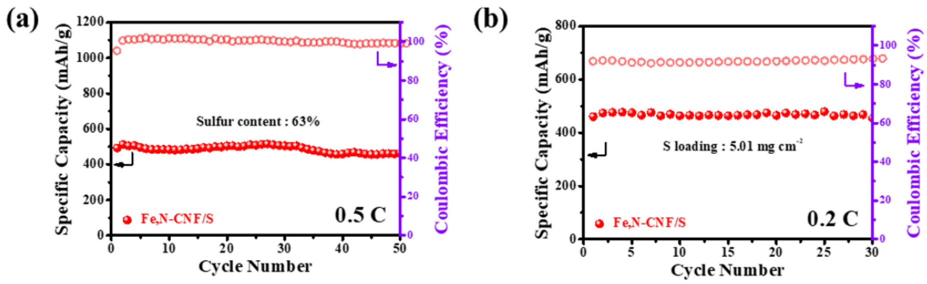

Fig.S11 Cycle analysis of electrodes with increased (a) sulfur content and (b) sulfur loading for practical application in Li-S batteries (LSBs).

Table S1. Comparison of studies applying ZIF-based fibers and ZIF-derived CNF in lithium-sulfur batteries (LSBs)

Samples	Synthesis Methods		Properties	Reference
	Electrospinning	In-situ Growth		
Fe/N-CNF	O (Fe-seed Contained)	O (2-STEP Growth)	✓ Using a two-step nucleation-growth process with high surface polarity and exposed active sites enhances strong chemisorption.	This Work
FeSA-PCNF	O	X	✓ A lightweight, flexible architecture with a hierarchical porous structure.	1
FeZn-PCNF	O	X	✓ A carbon fibrous network prov ideshigh conductivity while en hancingphysical immobilizatio n.	2
FeSA-NC@CBC	X	O (Solvoth ermal)	✓ A hierarchical porous structure is achieved using bacterial cellulose (BC) for enhanced functionality.	3
CNF/Co-Co_9S_8-NC	X	O (Solvothermal)	✓ 3D Hyperfine Carbon Nanofibers Synthesized Using Bacterial Cellulose (BC).	4
CoS_2-SPAN-CNT	O (Ligand Contained)	O	✓ SPAN Composite Structures Designed to Suppress Volume Expansion.	5

Table S2 Comparison of specific surface areas and average pore sizes of CNF structures used in LSBs

Samples	Surface Area [m^2 g^{-1}]	Average Pore Size [nm]	Reference
B_4C@CNF	34.4	3.85	[1]
SnS_2@HCNF	34.2	9.76	[2]
Fe_3C/N-CNF	13.8	-	[3]
Mn_3O_4@CNF	40.0	-	[4]
CNF/rGO	43.8	-	[5]

Table S3. Comparison of the bond lengths of Fe-S and Li-N in the structure after adsorption

Samples	Fe-S bond length (Å)	Li-N bond length (Å)	Li-C bond length (Å)
Graphene-Li_2S	-	-	2.330
NC-Li_2S	-	2.122	-
FeNC-Li_2S	2.347	2.116	-

Table S4 Comparison of Li-ion diffusion coefficients for Fe/N-CNF/S and N-CNF/S measured from A1, C1, and C2 peaks in CV profiles

Samples	D_{Li+} [cm^2 s^{-1}]		
	A1	C1	C2
Fe/N-CNF/S	$6.26x10^{-8}$	$1.58x10^{-8}$	$1.62x10^{-8}$
N-CNF/S	$3.04x10^{-8}$	$0.49x10^{-8}$	$1.54x10^{-8}$

Table S5. Electrochemical performances of Fe/N-CNF/S cathode with the reported literature

Samples	Sulfur Contents [%]	Initial Capacity [mAh g^{-1}]	Capacity Retention [%]	Reference
Fe/N-CNF/S	70	620 (2.0 C)	78 (200 Cycle)	This work
Co@NCNTs-2	77	578 (0.5 C)	79 (300 Cycle)	[6]
CoFe@SnCNF/S	85	611 (0.5 C)	76 (200 Cycle)	[7]
HSAC-S@CF	66	1100 (0.06C)	56 (100 Cycle)	[8]
OM-Mn_2O_3/S	60	998 (0.5 C)	56 (250 Cycle)	[9]

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