Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Bifunctional semi-closed YF_3-doped 1D carbon nanofibers with 3D porous network structure including fluorinating interphases and polysulfide confinement for lithium-sulfur battery

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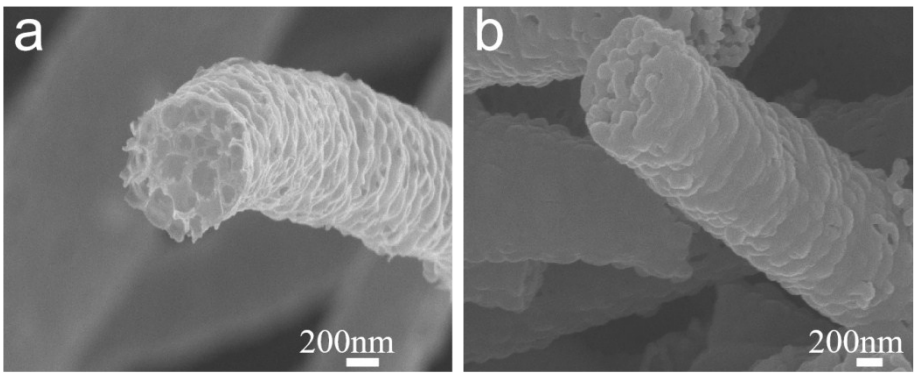

Figure S1 Cross section diagram of Y-2 before (a) and after (b) sulfur loading

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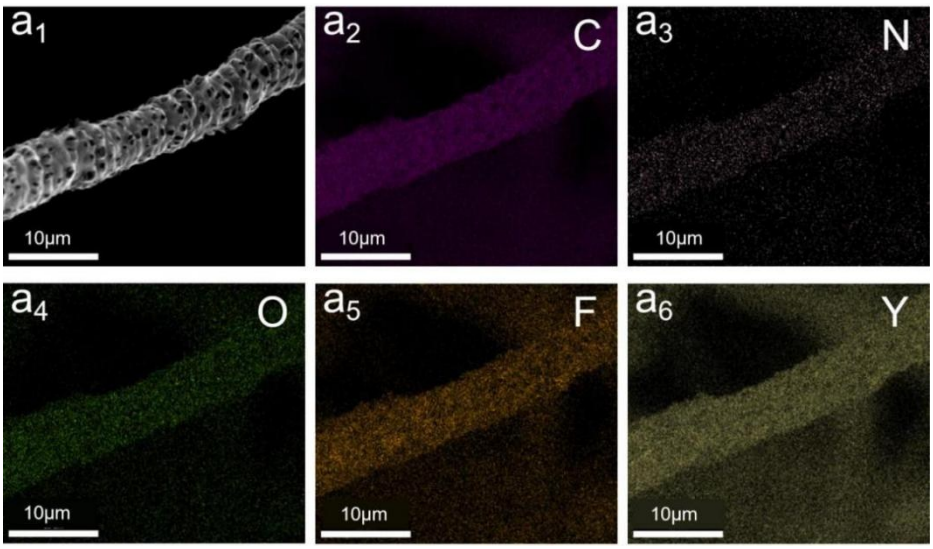

Figure S2 C, N, O, F and Y EDX mapping of SEM images for Y-2.

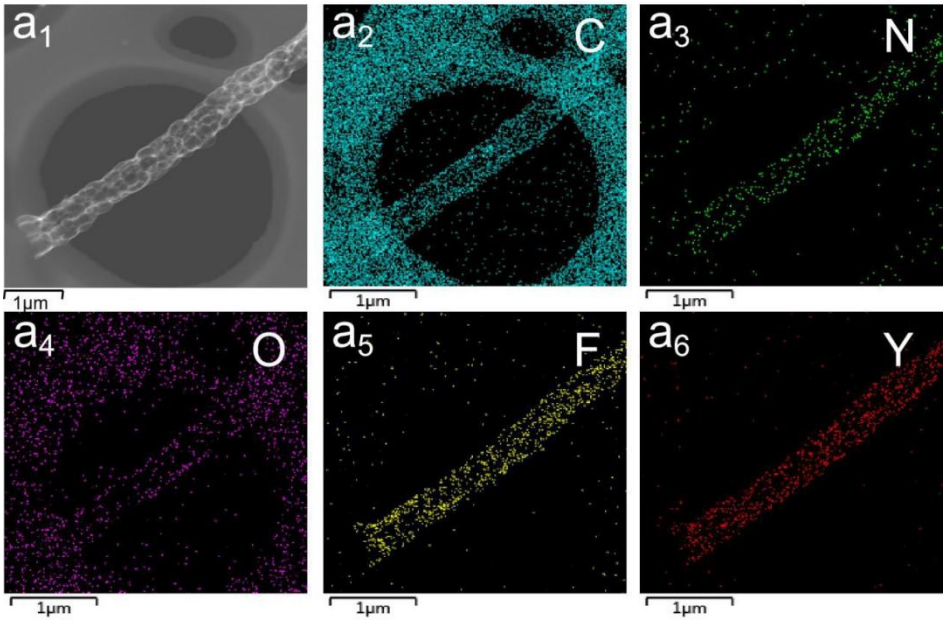

Figure. S3 C,N,O,F and Y EDX mapping of HR-TEM images for Y-2.

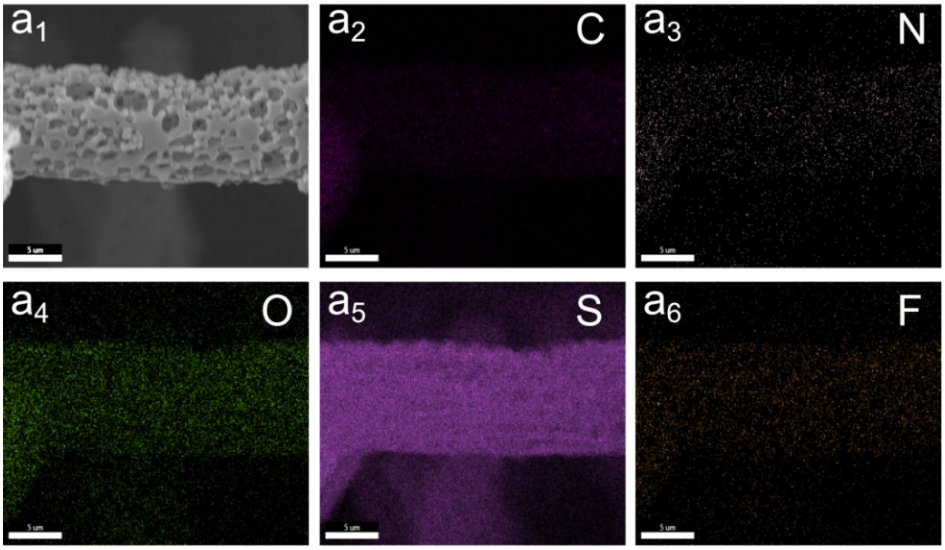

Figure. S4 C,N,O,F and S EDX mapping of SEM images for Y-0-S.

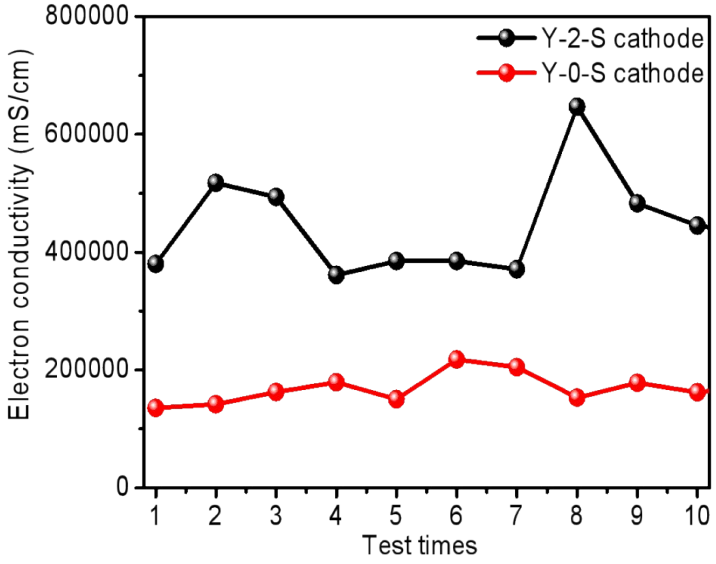

Figure S5 Electron conductivity of cathode sheets of Y-2-S and Y-0-S.

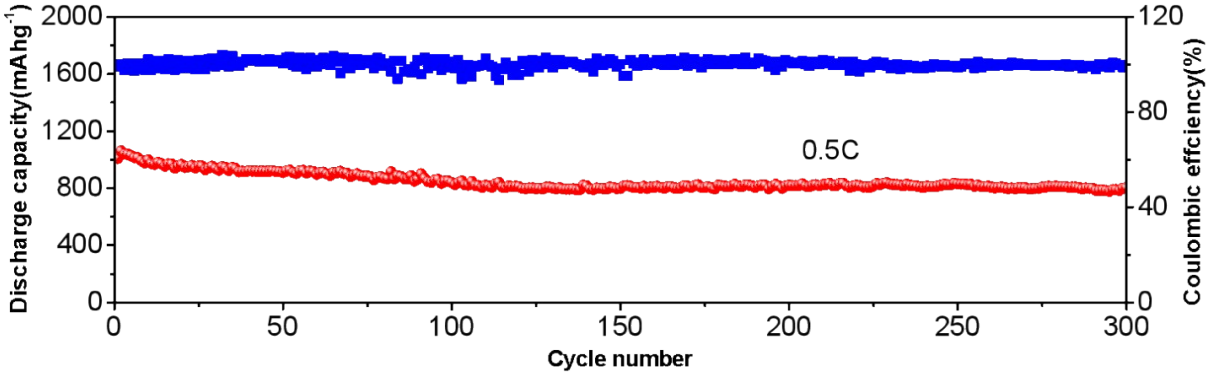

Figure S6 Long term cycling performance of cathodes with Y-2 at 0.5 C.

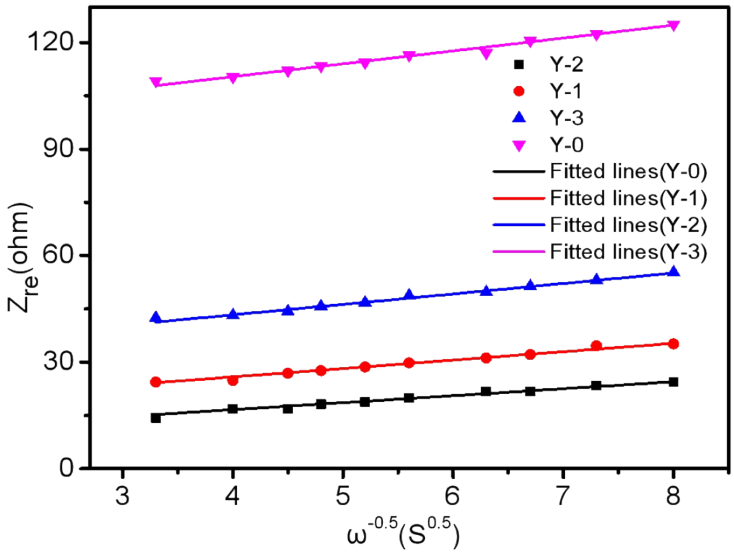

Figure S7 the relationship between Z_{re} and $\omega^{-0.5}$ at low frequencies

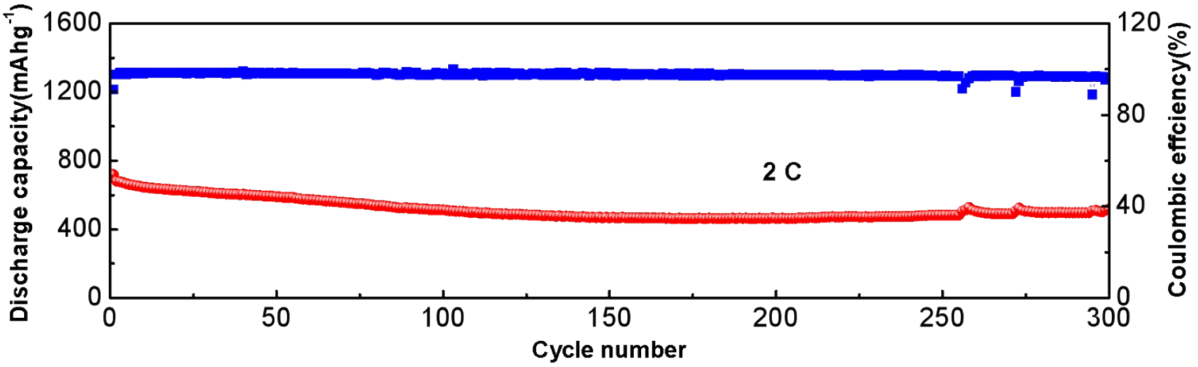

Figure S8 Thelong term cycling performance of Y-2 electrode with sulfur loading of 2.1 mg/cm^2 at 2 C.

Table S1 The electron conductivity, specific surface area and pore volume of CNFs with different YF_3 content

The content of YF_3	Y-1	Y-2	Y-3	Y-2-S
Specific surface area(m^2/g)	369.9	486.5	285.6	19.54
Pore volume(cm^3/g)	1.104	2.717	1.460	0.235
Electron conductivity (mS/cm)	78125	72993	54348	

Table. S2 Comparison of cycling stability of various representative carbon materials as sulfur cathodes for Li-S batteries

Sulfur cathode Materials	Sulfur Loading (wt.%)	Discharge Current rate	Cycles	Discharge Capacity (mAh g^{-1})	Capacity Loss Per Cycle(%)	Year	Ref.
3D nitrogen-doped porous carbon	54	1 C	500	541.7	0.067	2019	[S1]
Carbon matrix	60	0.5 C	400	511	0.110	2017	[S2]
Mesoporous Tio_2-Carbon nanotubes	65	0.5 C	500	577	0.070	2019	[S3]
3D printed sulfur-carbon composite	60	1 C	200	877.8	0.065	2019	[S4]
Well-architected porous N-doped carbon/Mno coaxial nonotubes	75	1 C	520	832	0.034	2019	[S5]
Hierarchically structured carbons	63	0.5 C	200	801.3	0.209	2018	[S6]
Cobalt-embedded N-doped porous carbon	70	1 C	200	633	0.105	2018	[S7]
Hollow carbon nanofibers with closed ends	60	2 C	500	620	0.078	2018	[S8]
Cobalt and porous Graphitic carbon	70	1 C	100	712	0.051	2018	[S9]
MOFS-derived nitroged-doped porous carbon grow on graphene	64	1 C	300	608	0.043	2018	[S10]
Electrospun TiO_2-impregnated hollow carbon nanofibers	65	2 C	340	458	0.056	2018	[S11]
Bamboo-Like Nitrogen-Doped Carbon Nanotubes	61.2	0.5 C	100	684.1	0.159	2017	[S12]
Graphitized carbon	90	0.1 C	100	739	0.186	2017	[S13]
MoS2-C nanohybrids	79.6	0.5 C	300	799.3	0.070	2018	[S14]
Hierarchical pore-structured CNT	70	2 C	100	734.1	0.290	2018	[S15]
Double-shelled Nio-$NiCO_2O_4$ heterostructured@carbon	73	0.5 C	500	716.9	0.059	2018	[S16]
CeF_3-doped porous carbon nanofibers	75	1 C	500	567.1	0.103	2018	[S17]
3D CoO/Co activated free-standing porous carbon fiber	61.2	0.5 C	100	684.1	0.159	2018	[S18]
SC-YF3 doped-3D in 1D CNFs	80	2 C	800	579.7	0.029		**This work**

Table S3 The Warburg diffusion coefficients values (σ_w) and the diffusion coefficient values of the lithium ions (D) for CNFs with different YF3 content

The content of YF_3	Y-0	Y-1	Y-2	Y-3
σ_w (Ω $s^{-0.5}$)	3.63	2.36	1.96	2.94
D (cm^2 s^{-1})	1.3×10^{-9}	3×10^{-9}	4.4×10^{-9}	1.9×10^{-9}

The inclined line is attributed to the diffusion of the Li^+ into the bulk of the electrode material named as Warburg diffusion. The Warburg diffusion coefficients values (σ_w) can be obtained by formula (1)

$$Z_{re}=R_s+R_{ct}+\sigma_w\omega^{-0.5} \quad (1)$$

σ_w are the slopes for the plots of Z_{re} vs. the reciprocal root square of the lower angular frequencies ($\omega^{-0.5}$), which are presented in **Figure S7** [19]. The diffusion coefficient values of the lithium ions (D) for its diffusion into the bulk electrode materials have been calculated using formula (2) and are listed in **Table S3** too [20].

$$D=0.5(R_T/AF^2\sigma_wC)^2 \quad (2)$$

where R is the gas constant (8.314 J mol^{-1} K^{-1}), T is the room temperature (298.5 K), A is the area of the electrode surface (1.35 cm^2), F is the Faraday's constant (9.65×104 C mol^{-1}) and C is the molar concentration of Li^+ ions (1.1×10^{-3} mol cm^{-3}).

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