Electronic Supplementary Information

Enveloping Ultrathin Ti_3C_2 Nanosheets on Carbon Fibers: A High-Density Sulfur Loaded Lithium-Sulfur Battery Cathode with Remarkable Cycling Stability

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1. SUPPORTING FIGURES

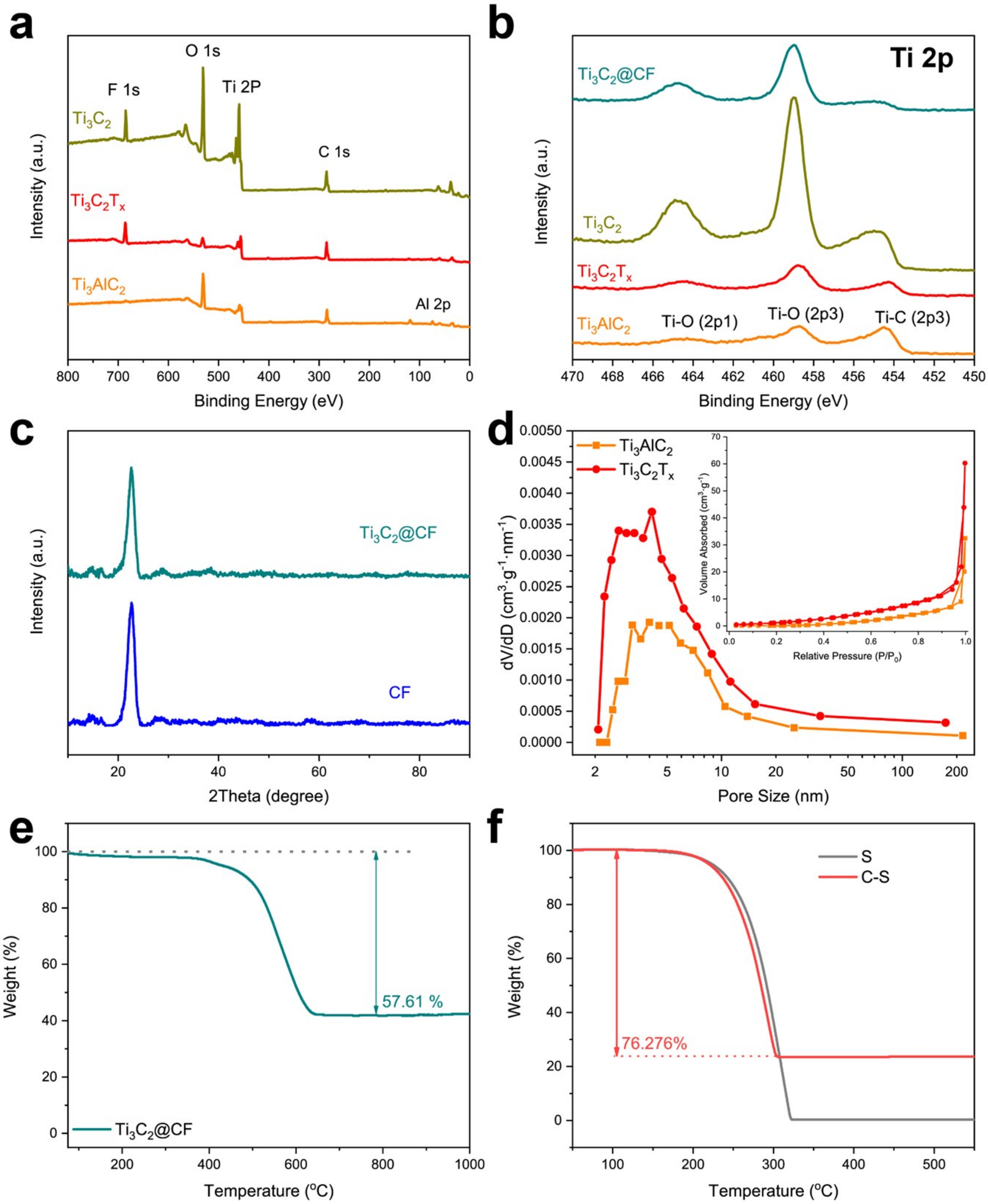

Figure S1. (a) XPS survey spectrum of Ti_3AlC_2, Ti_3C_2Tx, and Ti_3C_2. (b) High-resolution Ti 2p XPS spectra of Ti_3AlC_2, Ti_3C_2Tx, Ti_3C_2 and Ti_3C_2@CF. (c) XRD patterns of Ti_3C_2@CF and CF. (d) Pore distributions and N_2 adsorption and desorption isotherms plots (inset) of Ti_3AlC_2 and $Ti_3C_2T_x$. (e) TGA curves of CF, $Ti_3C_2T_x$ and Ti_3C_2@CF from room temperature to 1000°C in the air atmosphere. (f) TGA curves of C-S composite from room temperature to 600°C in Nitrogen atmosphere.

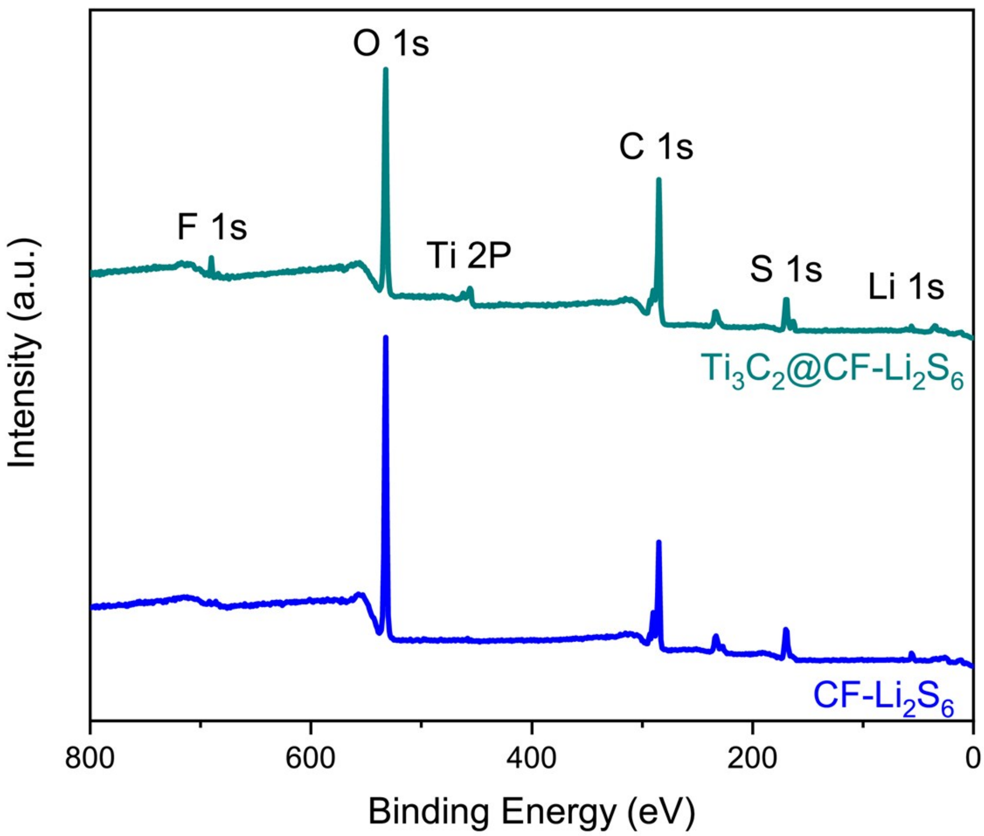

Figure S2. XPS survey spectrum of Ti_3C_2@CF-Li_2S_6 composites and CF-Li_2S_6 composites.

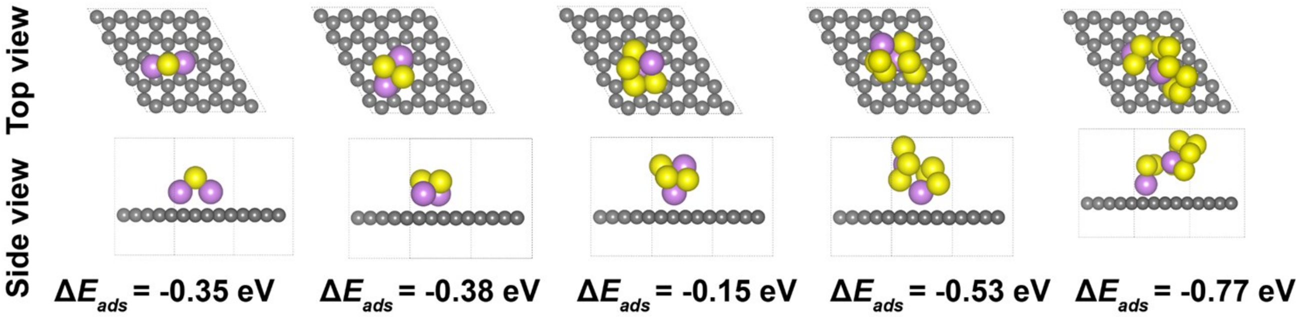

Figure S3. Optimized geometries of the most stable Li_2S_n on graphene supercell model surfaces and corresponding adsorption energies, respectively.

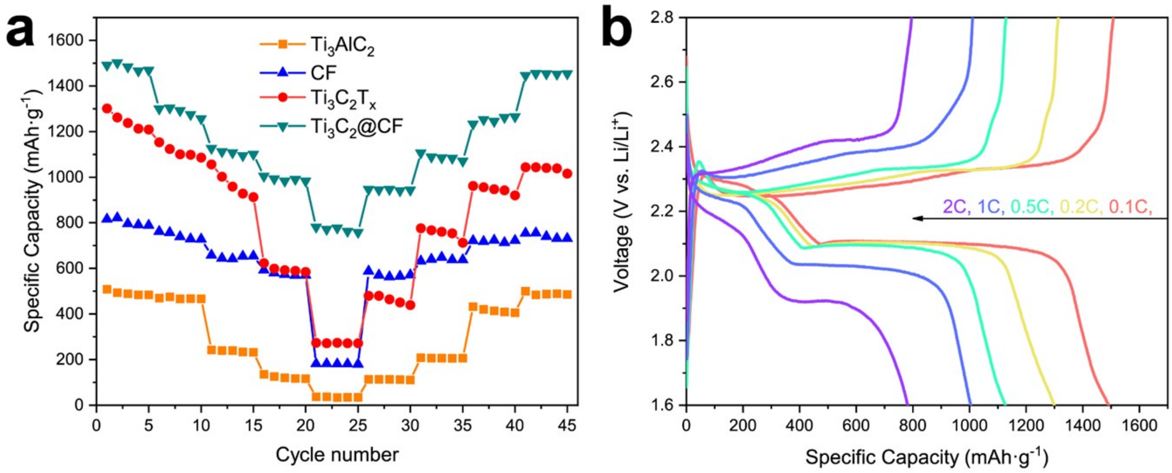

Figure S4. (a) Cycling performance of Ti_3AlC_2-S, CF-S, $Ti_3C_2T_x$-S, and Ti_3C_2@CF-S cathodes at different rates from 0.1 C to 2 C. (b) galvanostatic charge-discharge curves of Ti_3C_2@CF-S cathodes at different rates from 0.1 C to 2 C

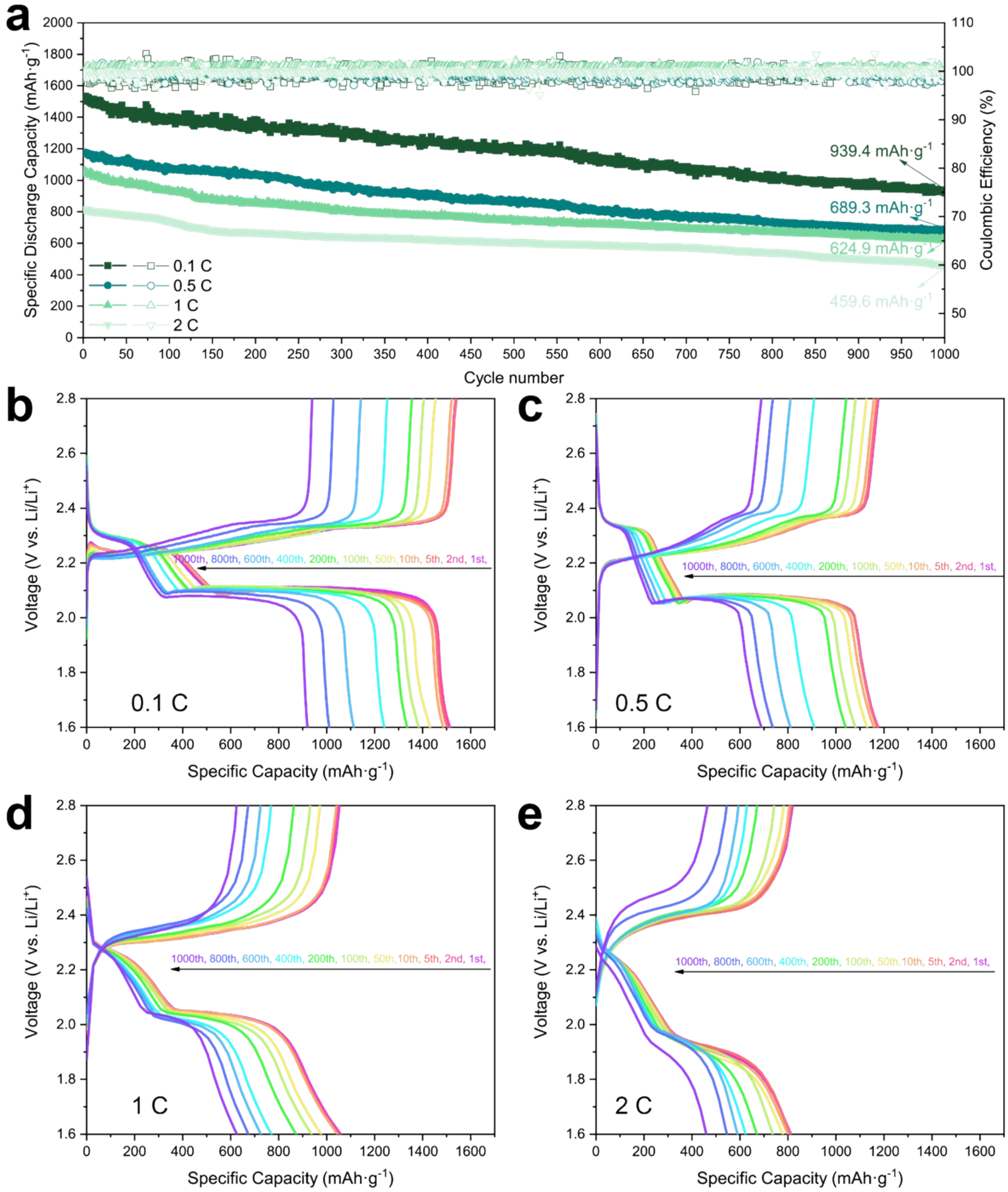

Figure S5. (a) Long cycling performance (1000 cycles) of Ti_3C_2@CF-S cathode with S loading of 4 mg·cm^{-2} at 0.1 C, 0.5 C, 1C, and 2 C, respectively. Galvanostatic charge-discharge curves of Ti_3C_2@CF-S cathode at (b) 0.1 C, (c) 0.5 C, (d) 1 C and (e) 2 C.

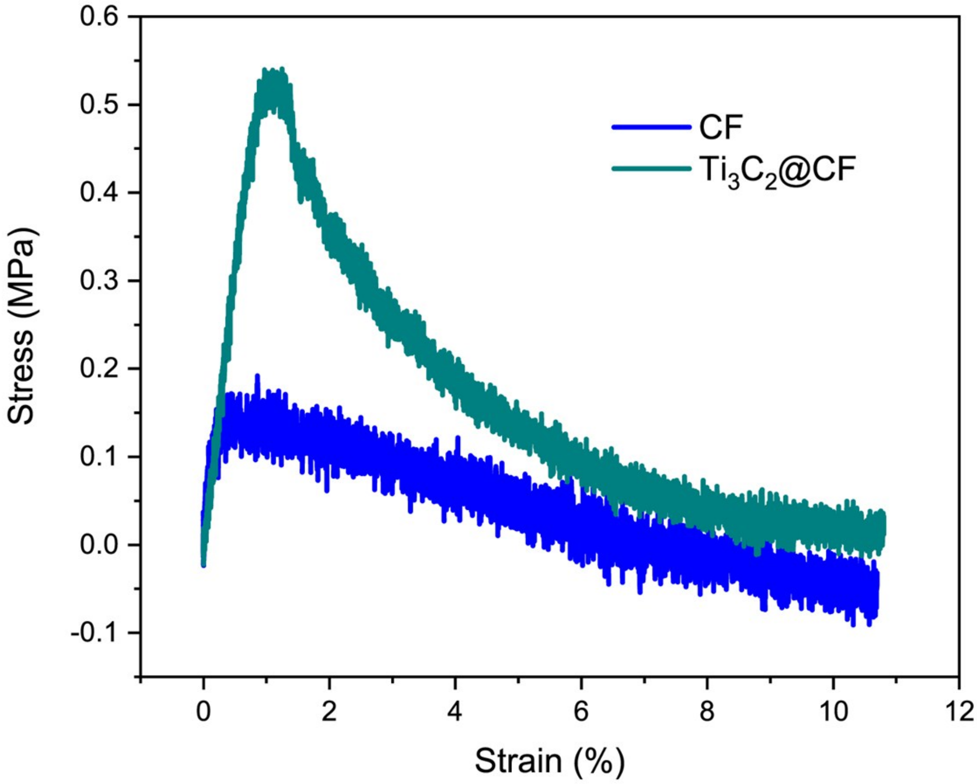

Figure S6. Stress-strain curves of CF and Ti_3C_2@CF.

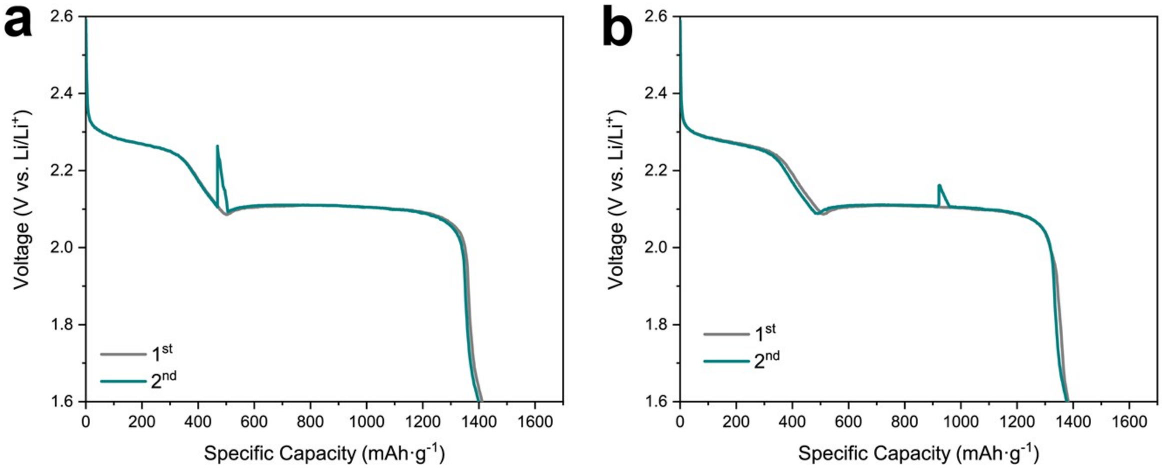

Figure S7. Galvanostatic discharge curves of Ti_3C_2@CF-S cathode with S loading of 4 mg·cm^{-2} at 0.2C: (a) 1/3 and (b) 2/3 charge retention test.

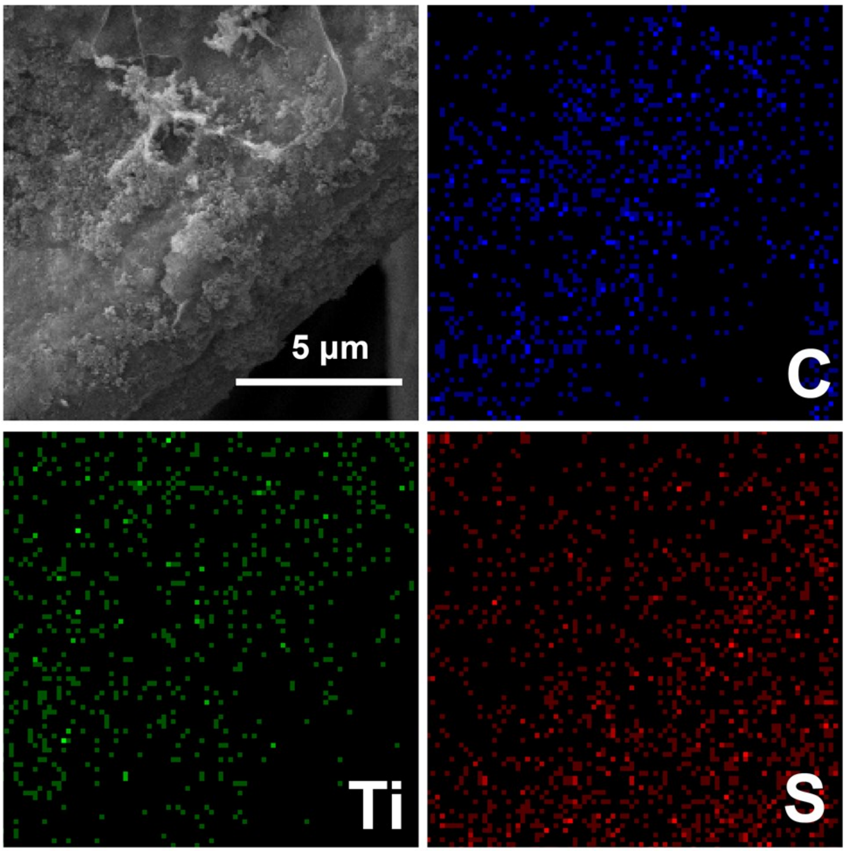

Figure S8. SEM image of Ti_3C_2@CF-S cathode before cycling, and the corresponding elemental mapping images of C, Ti and S.

2.SUPPORTING TABLES

Table S1. Computed adsorption energies (eV) of Li_2S_x on Ti_3C_2 (001) slab, Li_2S_x on graphene supercell

	Li_2S	Li_2S_2	Li_2S_4	Li_2S_6	Li_2S_8
$E_{Ti_3C_2}$	-697.37	-697.37	-697.37	-697.37	-697.37
$E_{Li_2S_x}$	-7.99	-13.01	-22.42	-30.31	-37.90
ΔE_{ads}	-5.20	-7.97	-5.89	>9 (Dissociated into S + Li_2S_5)	>9 (Dissociated into S + Li_2S_7)
$E_{graphene}$	-461.56	-461.56	-461.56	-461.56	-461.56
$E_{Li_2S_x}$	-7.99	-13.01	-22.42	-30.31	-37.90
ΔE_{ads}	-0.35	-0.38	-0.15	-0.53	-0.77

Table S2. Comparison of the performances between this work and other Li-S batteries corresponding to Figure 5f.

Sulfur host	Discharge current (C)	S loading ($mg \cdot cm^{-2}$)	Initial / highest capacity ($mAh \cdot cm^{-1}$)	Ref.
Ti_3C_2@CF	0.2	4	5.7	This work
		8	10.2	
		12	14.7	
VO_2(p)-V_2C	0.2	10.2	9.3	[1]
BiOCl/G	0.2	4.8	5.1	[2]
PTCDI/ G	0.2	4.48	4.5	[3]
ISCF	0.2	8	6.23	[4]
TiC@G	0.2	3.5	3.6	[5]
3DG/TM	0.1	10	11.8	[6]
Co-N/G	0.2	6	5.1	[7]
HFeNG	0.1	5	5	[8]
PCS-80	0.2	5.5	4.8	[9]
TiB_2	0.2	3.9	3.8	[10]

Table S3. Comparison of the performance between this work and other Li-S batteries.

Sulfur host	S loading ($mg·cm^{-2}$)	Current density (C)	Initial capacity ($mAh·g^{-1}$)	Cycle capacity ($mAh·g^{-1}$ /cycle)	Capacity decay ration (%)	Retention ration (%)	Ref.
Ti_3C_2@CF	4	0.1	1512.7	920.1 (1000^{th})	0.04	60.82	This work
		0.5	1175.2	689.2 (1000^{th})	0.04	58.64	
		1	1058.4	626.0 (1000^{th})	0.04	59.14	
		2	812.2	459.6 (1000^{th})	0.04	56.58	
Hierarchical Porous Carbon	1	0.3	998	899 (100^{th})	0.10	90.08	[11]
Ti_4O_7	0.9	2	850	595 (500^{th})	0.06	70.00	[12]
N and S dual-doped carbon	1.7	0.5	1135	775 (500^{th})	0.06	68.28	[13]
3D mesoporous Graphene	2.4	1	1187	852 (500^{th})	0.06	71.78	[14]
Titanium monoxide @carbon hollow spheres	1.5	0.2	1190	750 (500^{th})	0.07	63.03	[15]
TiC@G	3.5	0.2	1032	670 (100^{th})	0.35	64.92	[5]
TiO_2 deposited on N-doped graphene	1.8	1	1069.5	918.3 (500^{th})	0.03	85.86	[16]
Quinonoid imine-doped graphene	1.4	1	953	605 (500^{th})	0.07	63.48	[17]
Co_9S_8 inlaid carbon hollow nanopolyhedra	3	0.5	890	680 (300^{th})	0.08	76.40	[18]
Co_4N	2	2	882	761 (1000^{th})	0.01	86.28	[19]
CMK-3@ PANS@TPS	2.1	1	994	698 (1000^{th})	0.03	70.22	[20]
Molecularly imprinted polymer	1.5	0.5	1059	826 (150^{th})	0.15	78.00	[21]
Graphene@cucurbi	4.2	0.1	900	800 (90^{th})	0.12	88.89	[22]

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CO_3S_4	2.5	1	953	610 (450th)	0.08	64.01	[23]
Coupled NiS and hollow carbon spheres	2.3	0.5	723	695 (300th)	0.01	96.13	[24]
$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$	1.1	0.5	793	632 (400th)	0.05	79.70	[25]
TiB_2	3.9	0.2	965	837 (100th)	0.13	86.74	[10]
Porous carbon sheets	1.5	0.2	1344	1017 (50th)	0.49	75.67	[9]
Black phosphorus quantum dots	2	0.1	1234	1072 (200th)	0.07	86.87	[26]
MoN-VN	3	2	708	467 (500th)	0.07	65.96	[27]

3. SUPPORTING REFERENCES

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