Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

Defective MOF Architecture Threaded by Interlaced Carbon Nanotubes for High-Cycling Lithium-Sulfur Batteries

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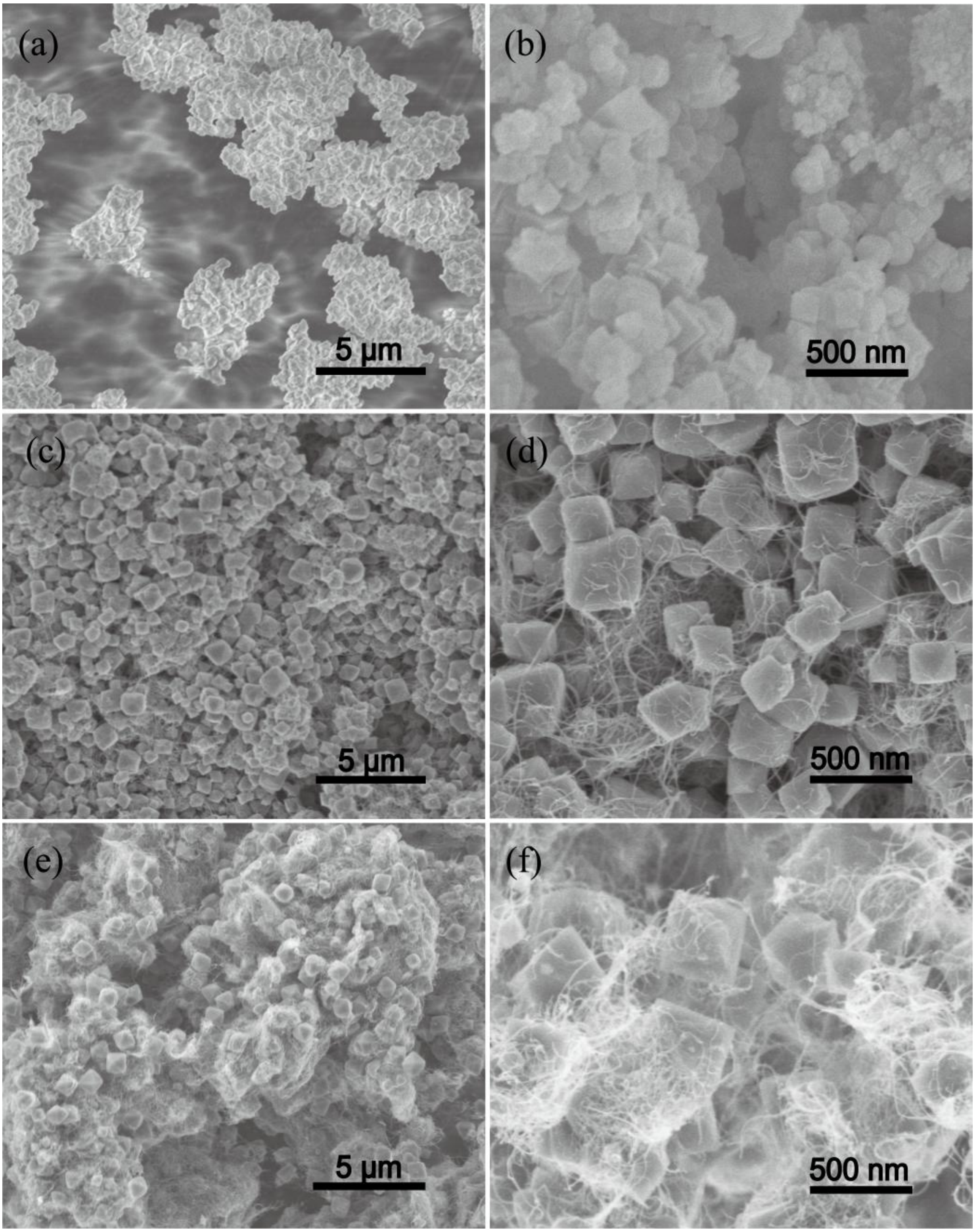

Fig. S 1 SEM morphologies of (a) and (b) Uio-66, (c) and (d) UC-2, (e) and (f) UC-5

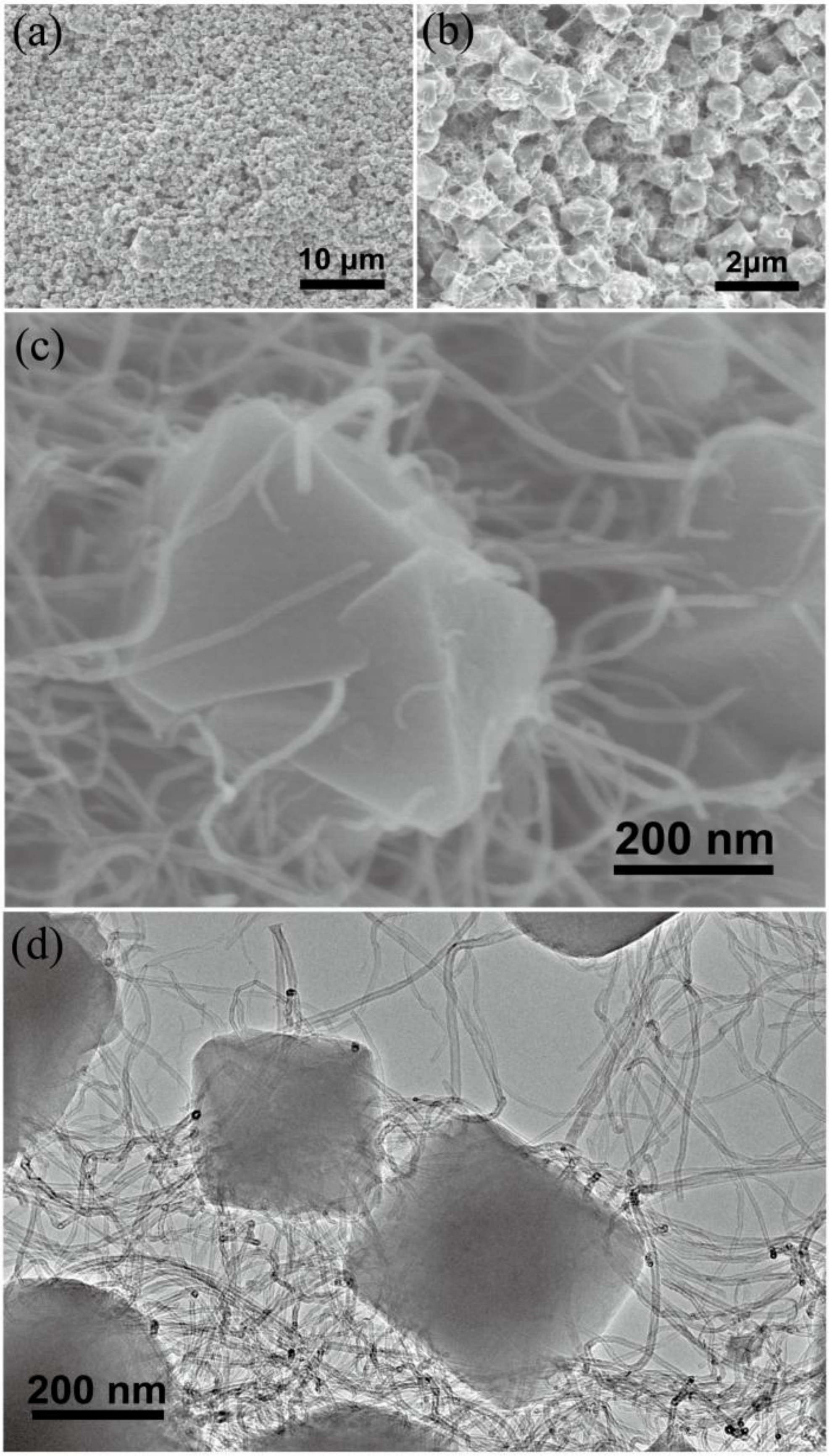

Fig. S 2 (a)-(c) SEM and (d) TEM photographies of UC-3 composite.

Table S 1 BET characteristics of CNTs, Uio-66, UC series and S@UC hybrid series and their pore volume and average pore diameters (except CNTs) derived from their 77K N_2 isotherms based on the nonlocal density function theory (NLDFT).

Samples	S_{BET} /($m^2 \cdot g^{-1}$)	V_{total} /($cm^3 \cdot g^{-1}$)	$D_{average}$ / (nm)
CNTs	278	0.72	12.3
Uio-66	1157	0.43	1.08
UC-2	976	0.47	1.33
UC-3	863	0.56	1.59
UC-5	738	0.53	1.64
S@UC-2	17.13	0.058	1.77
S@UC-3	15.36	0.031	1.85
S@UC-5	6.62	0.012	4.54

(Note that all data of CNTs are obtained from its BET characteristics)

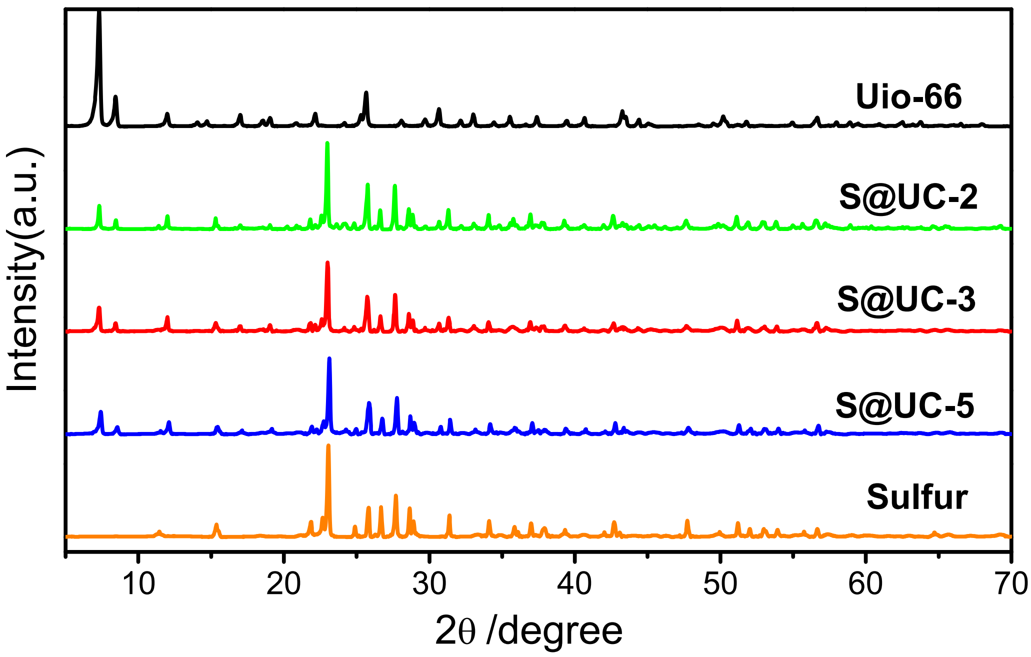

Fig. S 3 XRD patterns of Uio-66, S@UC series and sulfur.

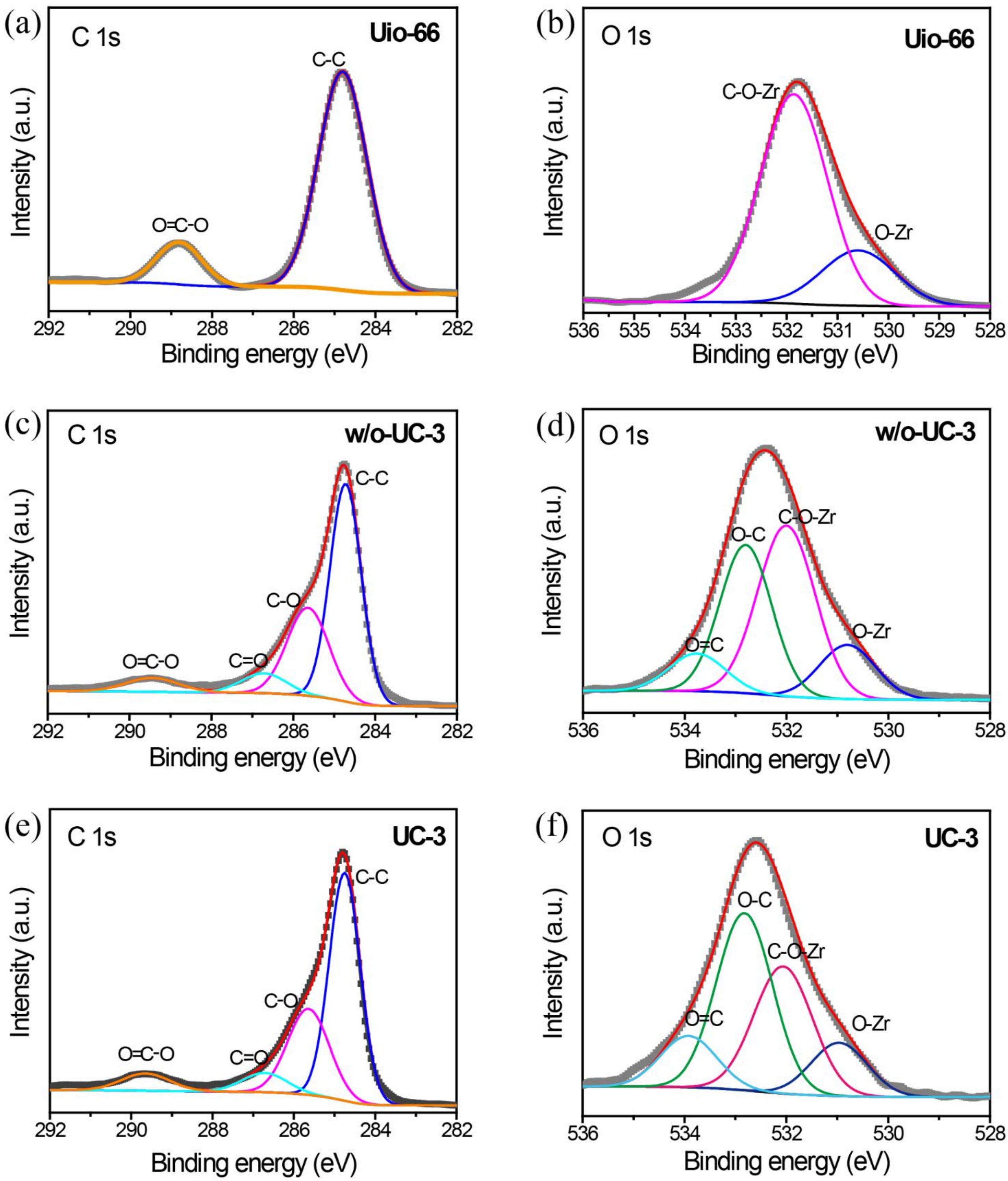

Fig. S 4 C 1s and O 1s XPS spectra of (a) and (b) Uio-66, (c) and (d) w/o-UC-3 and (e) and (f) S@UC-3, respectively.

Table S 2 Data obtained from the quantitative analysis for C 1s and O 1s spectra of w/o-UC-3 and UC-3.

Spectrum	Bond	Binding energy (eV)		Content (%)	
		w/o-UC-3	UC-3	w/o-UC-3	UC-3
C 1s	C-C	287.74	284.75	68.27%	67.37%
	C-O	285.62	285.64	19.01%	18.61%
	C=O	286.74	286.72	4.81%	4.78%
	O=C-O	289.46	289.64	7.91%	9.24%
O 1s	O-Zr	530.8	530.96	7.68%	7.93%
	Zr-O-C	532	532.06	29.09%	24.49%
	O-C	532.8	532.82	57.00%	58.34%
	O=C	533.76	533.92	6.24%	9.24%

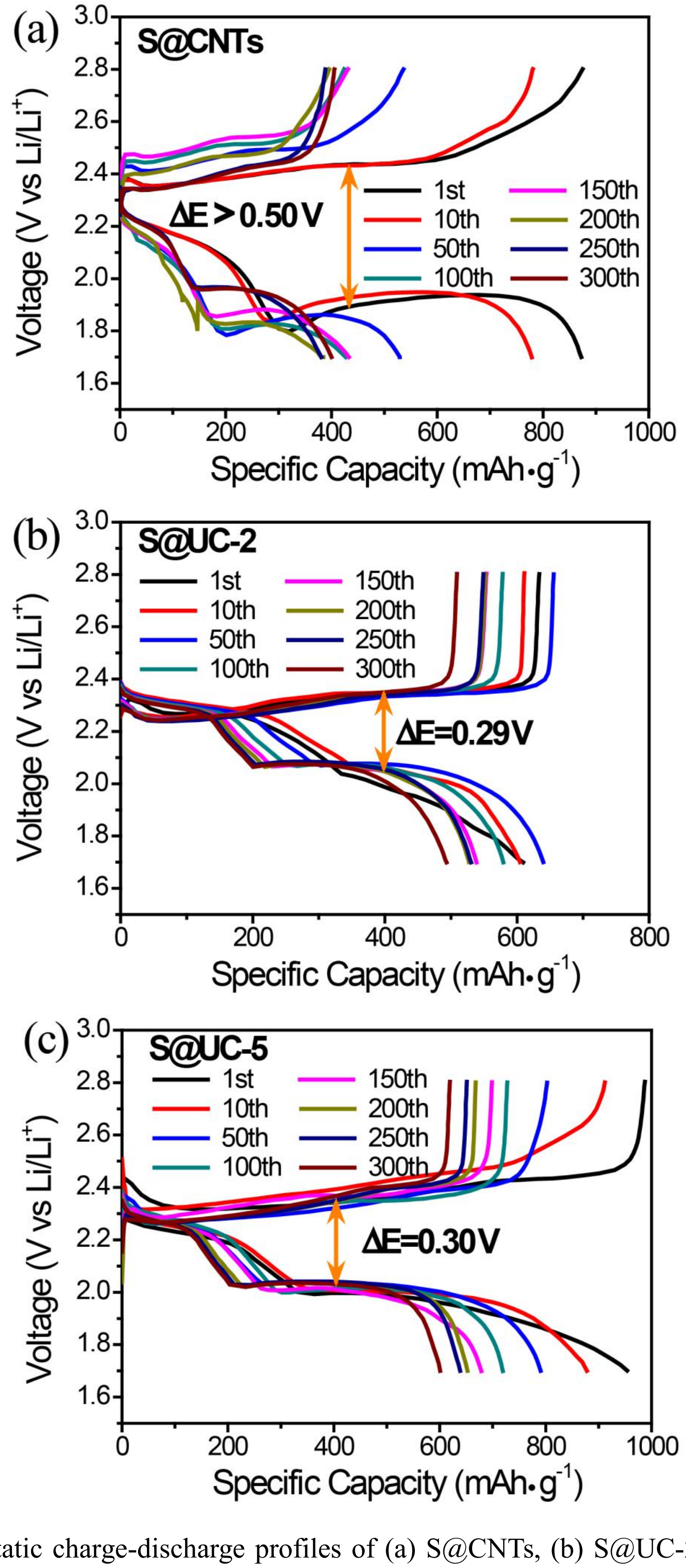

Fig. S 5 Galvanostatic charge-discharge profiles of (a) S@CNTs, (b) S@UC-2 and (c) S@UC-5 as the electrode at 0.5 $A \cdot g^{-1}$

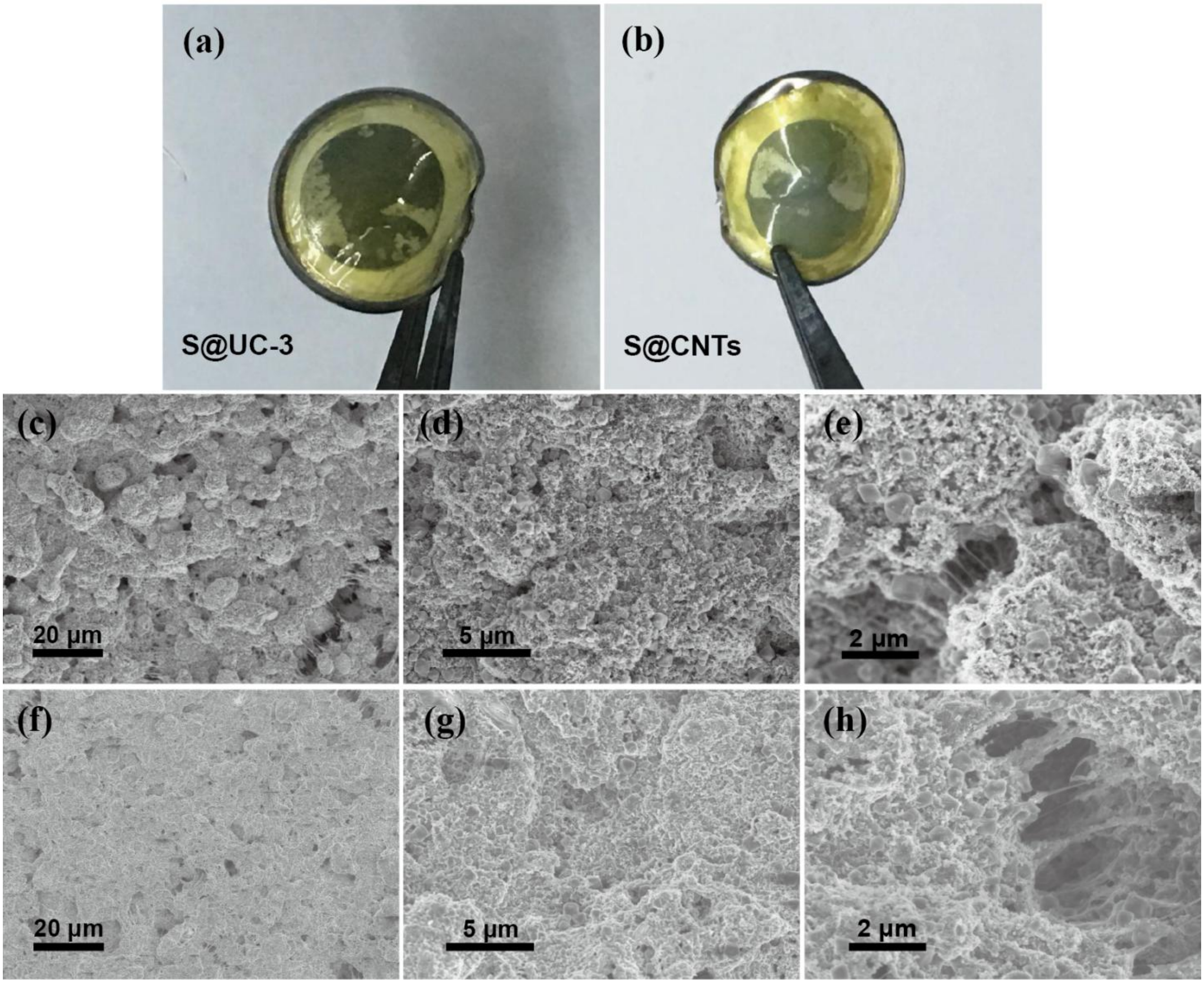

Fig. S 6 The disassemble cell pictures of (a) S@UC-3 electrode and (b) S@CNTs electrode after 300 cycles, conducted and obtained in the Ar gas filled glove box (O_2, H_2O<0.1 ppm) . The SEM images of (c)-(e) fresh and (f)-(h) cycled S@UC-3 electrode after 300 cycles cleaned by the DOL/DME (1:1) solvent.

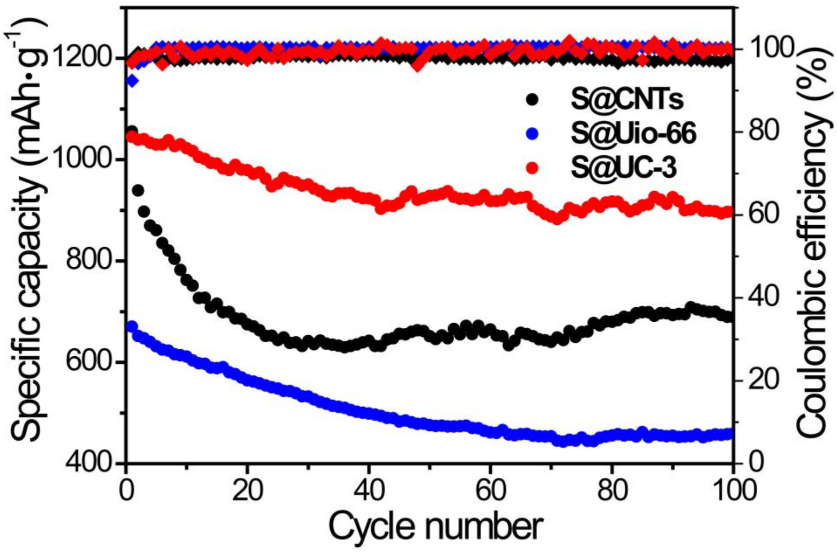

Fig. S 7 Cycling performance of the S@CNTs, S@Uio-66 and S@UC-3 electrodes at the current density of 0.1 $A\cdot g^{-1}$.

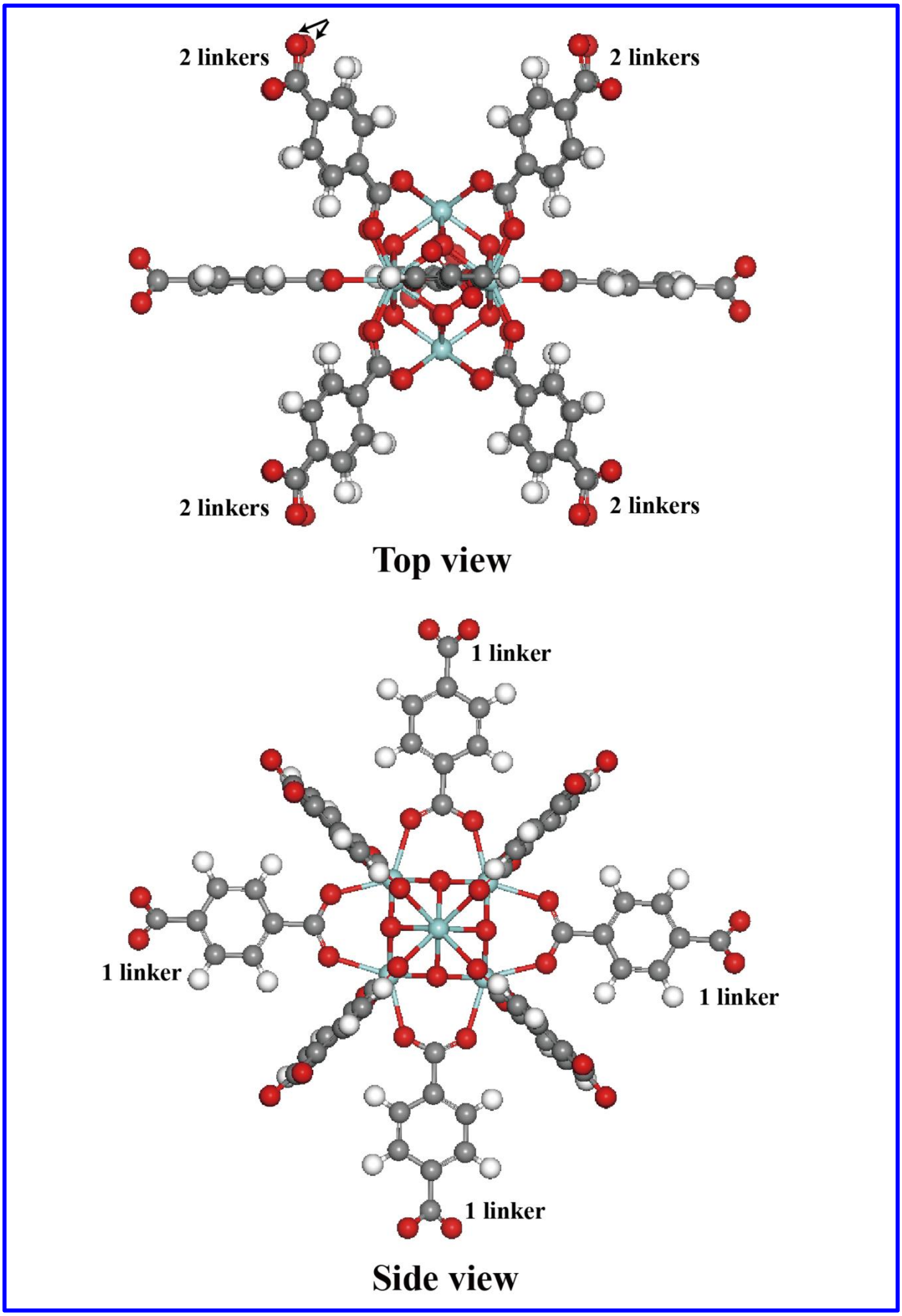

Fig. S 8 Atomic unit model configurations of the intact Uio-66 (top view and side view)

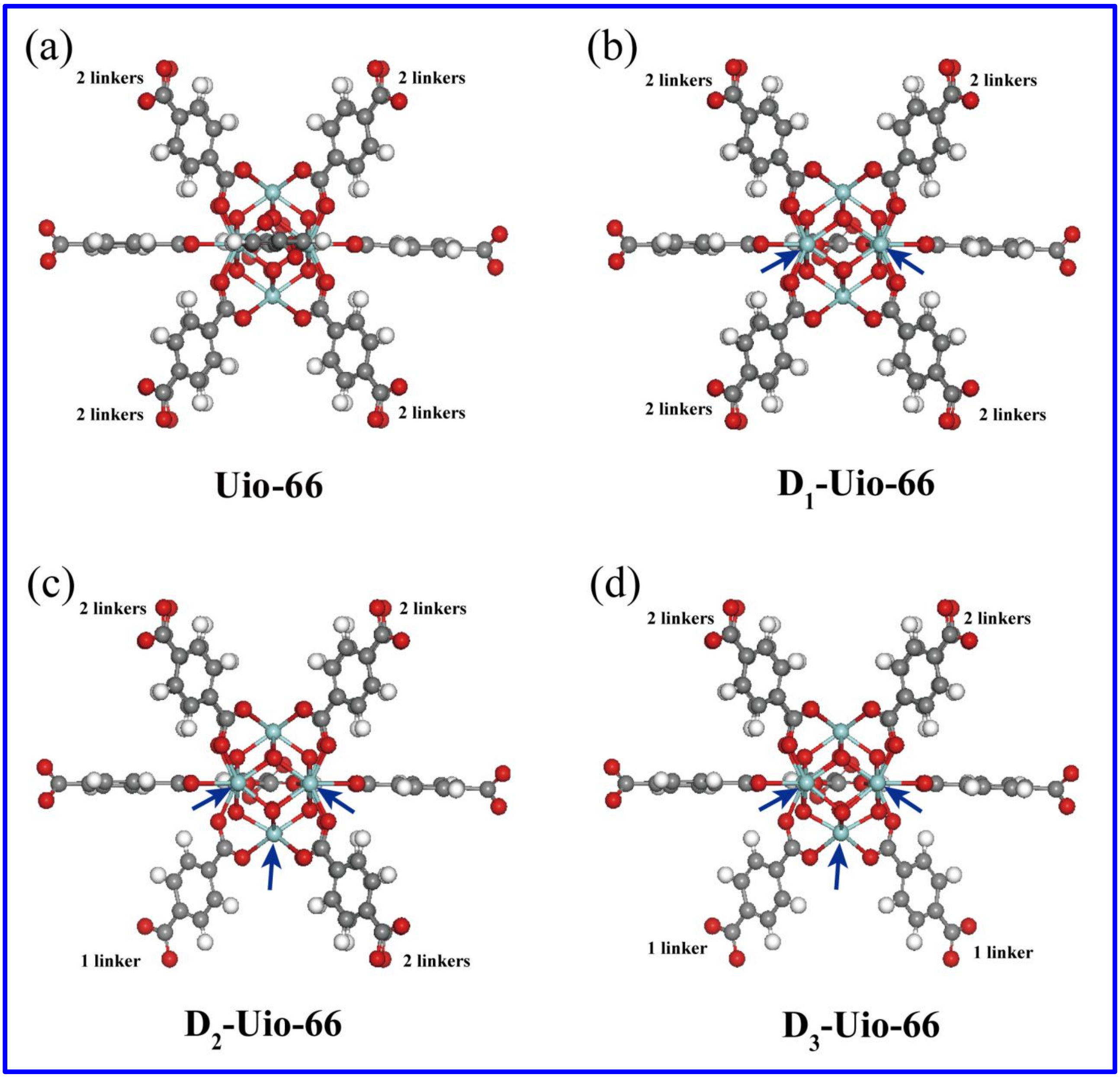

Fig. S 9 Atomic unit model configurations of (a) intact Uio-66 and (b)-(d) defective Uio-66 with one, two and three linker loss (denoted as D_1-Uio-66, D_2-Uio-66 and D_3-Uio-66). Gray, red, white and light blue spheres represent C, O, H and Zr atoms, respectively.

Table S 3 Performance comparisons of the representative MOFs-based sulfur electrodes (1C=1675 $mA·g^{-1}$).

Cathode	Sulfur content in the electrode	Potential range(V)	Maximum capacity ($mAh·g^{-1}$)	Average fading Rate	Discharge current density (Cycle number)	Ref.
S@UC-3	**~54%**	**1.7-2.8**	**1045**	**0.142%**	**100 $mA·g^{-1}$ (100)**	**This work**
			925	**0.055%**	**500 $mA·g^{-1}$ (300)**	
			764	**0.071%**	**1000 $mA·g^{-1}$ (800)**	
S@rGO/MIL100(Cr)	~ 41 %	1.0-3.0	869	0.200 %	0.1C (100)	1
S@ZIF-8	~ 30 %	1.8-2.8	793	0.101 %	0.5C (300)	2
S@Ni-MOF	~ 48 %	1.5-3.0	689	0.094 %	0.2C (200)	3
S@MOF-525(Cu)	~ 42 %	1.5-3.0	1200	0.207 %	0.2C (200)	4
S@rGO/MIL-100(V)	~ 35 %	1.6-3.0	849	0.170 %	0.1C (200)	5
S@HKUST-1/CNTs	~ 40 %	1.7-2.8	1263	0.080 %	0.2C (500)	6
S@nMOF-867	—	1.7-2.8	907	0.050 %	835 $mA·g^{-1}$ (500)	7
S@Cd-MOF	~ 50 %	1.5-2.8	1092	0.537 %	0.1C (50)	8

Note that average fading rate is calculated based on the formula:

$$\frac{(C_{Max}-C_{Ret})/C_{Max}}{N}\times 100\%$$

C_{Max} represents the maximum capacity, C_{Ret} represents the capacity retention after cycling, N represents the cycling numbers.

Table S 4 Cycling performance comparisons of UC-3 with several representative MOF-derived porous Carbon materials as the sulfur hosts for Li-S batteries

MOFs	Cathode	Sulfur content in the electrode	Potential range (V)	Maximum /Final Capacity ($mAh\cdot g^{-1}$)	Discharge current density (Cycle number)	Ref.
	S@UC-3	**~ 54%**	**1.7-2.8**	**925/765**	**500 $mA\cdot g^{-1}$ (300)**	**This work**
				764/486	**1000 $mA\cdot g^{-1}$ (800)**	
ZIF-8	GS-S/$C_{ZIF8\text{-}D}$	~ 38 %	1.0-3.0	1171/561	168 $mA\cdot g^{-1}$ (120)	[9]
	C-S-3	~ 22 %	1.0-3.0	1655/936	335 $mA\cdot g^{-1}$ (100)	[10]
	S/N3-C	~ 46 %	1.0-3.0	1500/800	0.1C (100)	[11]
	OCNTA/S	~ 56 %	1.7-2.6	1037/487	0.2C (1000)	[12]
	S/ZIF-8-NS-C	~ 56 %	1.7-2.8	887/587	0.5C (300)	[13]
ZIF-67	RGO/C-Co-S	~ 50 %	1.8-2.6	1218/949	300 $mA\cdot g^{-1}$ (300)	[14]
	NC-800-S60	~ 45 %	1.7-2.8	1124/511	800 $mA\cdot g^{-1}$ (400)	[15]
	S@Co-N-GC	~ 49 %	1.7-2.7	1440/850	0.2C (200)	[16]
MOF-5	MWCNT@Meso-C/S	~ 47 %	1.5-3.0	1343/540	0.5C (50)	[17]
	MCP-950/S	~ 63 %	1.8-2.8	1274/1041	0.2C (50)	[18]
	MPCN-S	~ 56 %	1.7-2.8	1000/740	0.5C (200)	[19]
	S-Zn-MOF	~ 35 %	1.7-2.6	1476/609	0.2C (200)	[20]
	GO@Meso-C/S	~ 64 %	1.8-2.7	1122/825	0.2C (100)	[21]
Al-MOF	S/FLHPC	~ 46 %	1.5-2.8	1100/751	0.5C (200)	[22]

Table S 5 Cycling stability comparisons of UC-3 with several representative polar materials as the sulfur host in Li-S batteries (1C=1675 mA·g^{-1}).

Polar host material	Sulfur content in the electrode	Fading rate	Discharge current density	Cycle number	Ref.
UC-3	**~ 54 %**	**0.055%**	**500 mA·g^{-1}**	**300**	**This work**
		0.071%	**1000 mA·g^{-1}**	**800**	
TiO_2	~ 53 %	0.033 %	0.5C	1000	23
Ti_4O_7	~ 48 %	0.060 %	2C	400	24
TiO	~ 56 %	0.082 %	0.5C	500	25
MnO_2	~ 56 %	0.028 %	0.5C	1500	26
VO_2	~ 60 %	0.058 %	0.5C	1000	27
Nb_2O_5	~ 48 %	0.146 %	0.5C	200	28
TiN	~ 50 %	0.070 %	0.5C	500	29
VN	~ 56 %	0.094 %	1C	200	30
TiS_2	~ 33% Li_2S	0.058 %	0.5C	400	31
CoS_2	~ 60 %	0.034 %	2C	2000	32
Co_3S_4	~ 53%	0.080 %	1C	450	33
Co_8S_9	~ 60 %	0.045 %	0.5C	1500	34
WS_2	~ 11 %	0.031 %	0.5C	500	35
MXene	~ 56 %	0.050 %	0.5C	650	36

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