Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Supporting Information

A New Ferrocene Covalent-based Organosulfur Cathode Material for High Stability Lithium-Sulfur Battery

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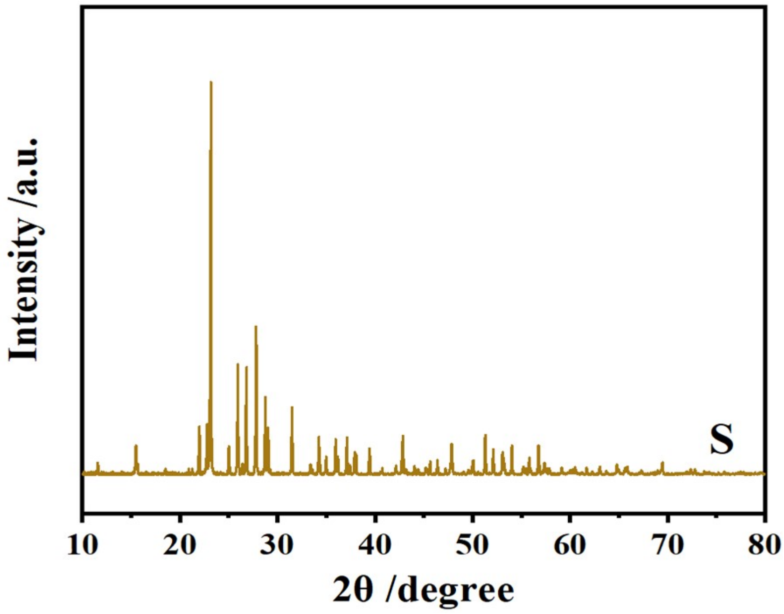

Fig. S1 The XRD analysis for sulfur.

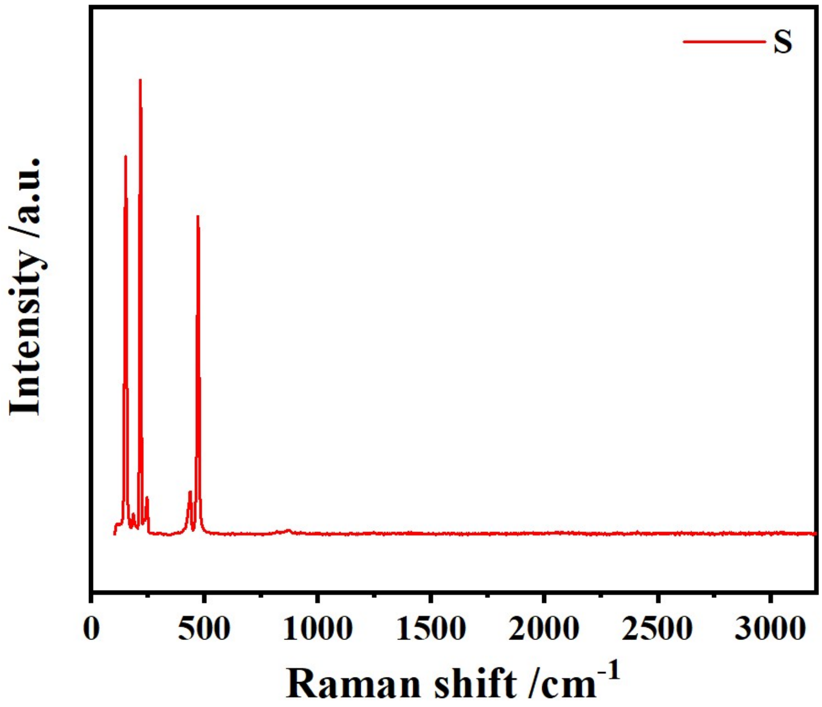

Fig. S2 The Raman spectrum of pure sulfur.

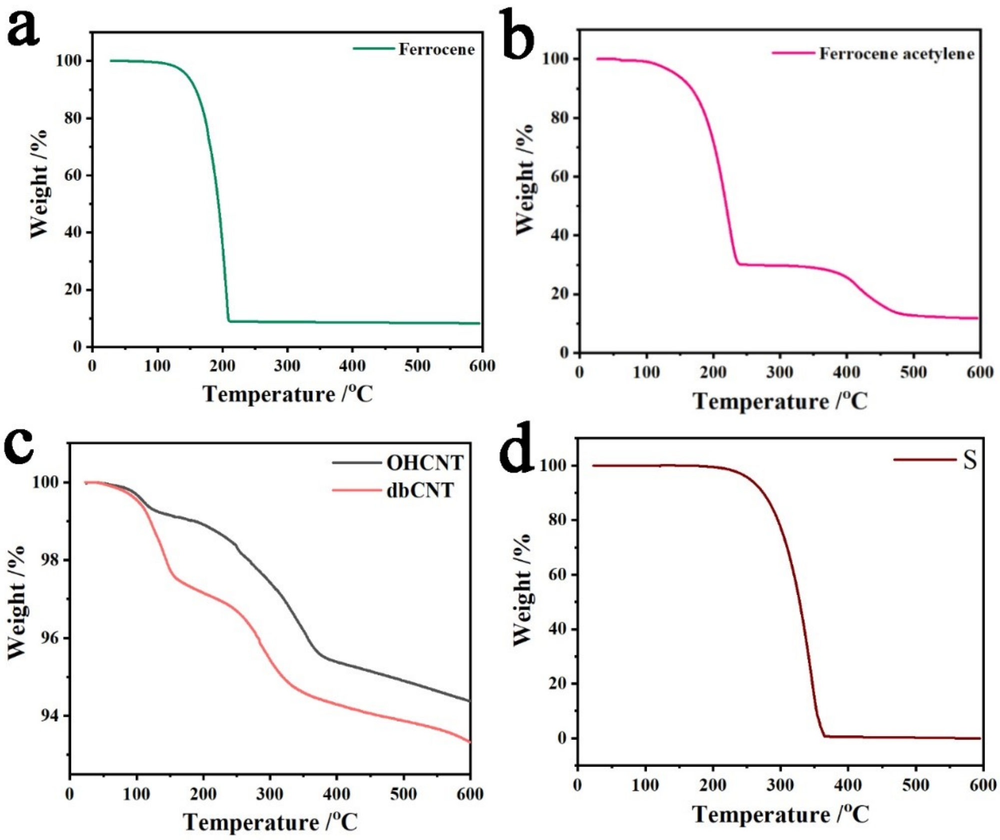

Fig. S3 The TGA analysis of ferrocene (a), ferrocene acetylene (b), OHCNT/dbCNT (c) and pure sulfur.

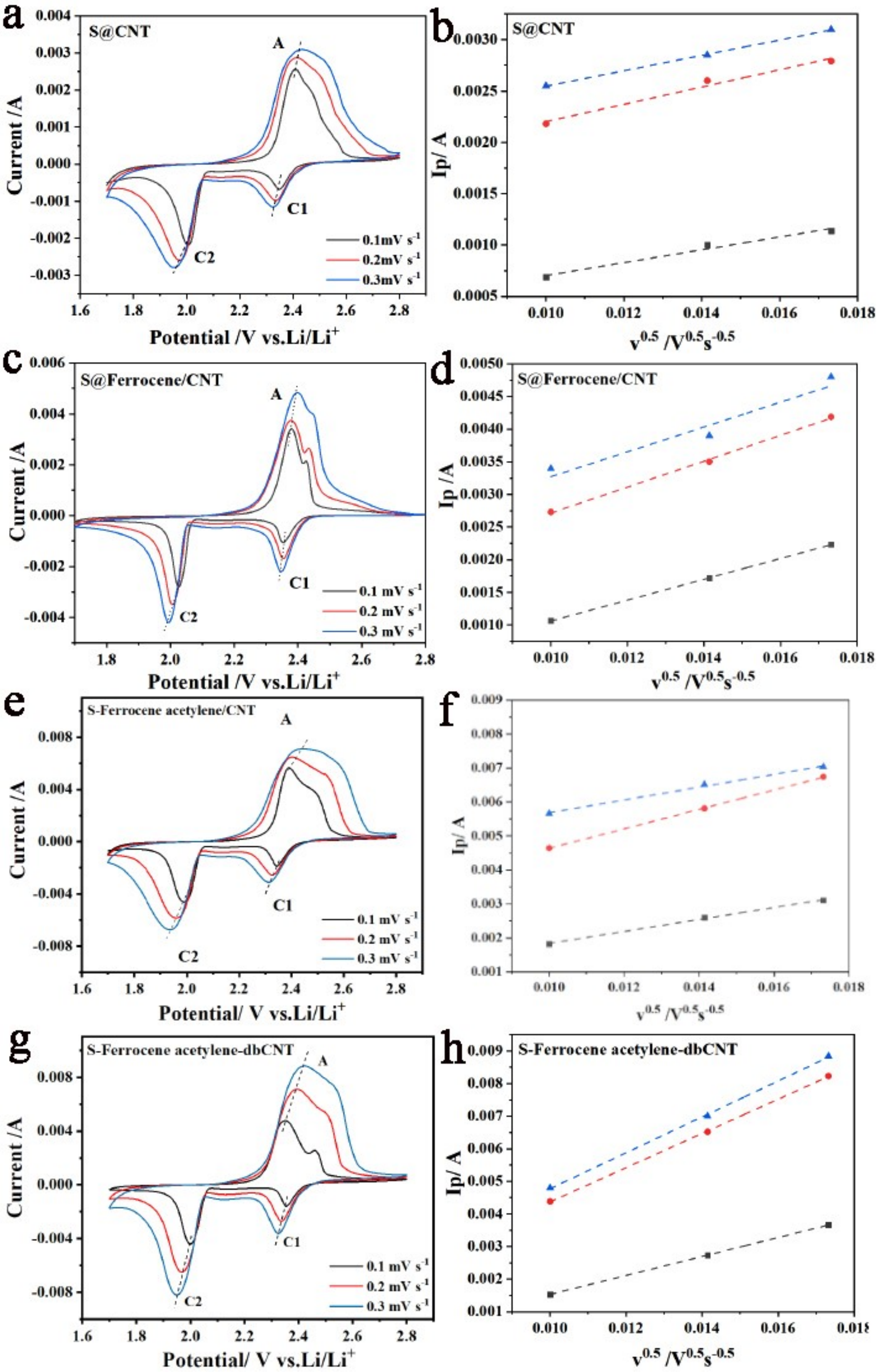

Fig. S4 The CV curves with different scan rates from 0.1 mV s^{-1} to 0.3 mV s^{-1} and linear fitting of the peak currents of CV curves for the cell with S@CNT (a-b), S@Ferrocene/CNT (c-d), S-Ferrocene/CNT (e-f) and S-Ferrocene acetylene-dbCNT (g-h) cathode.

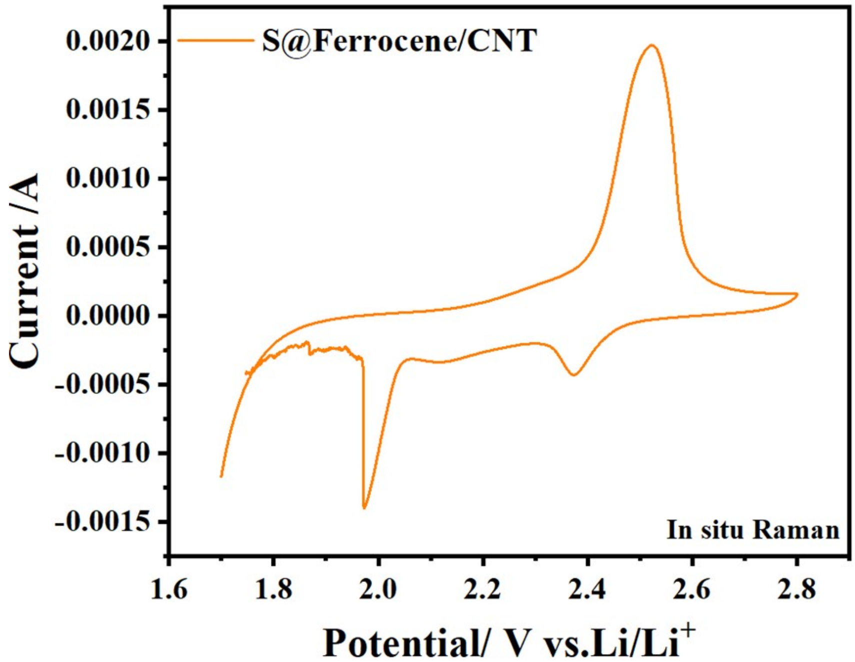

Fig. S5 (a) The CV curve of the mould with S@Ferrocene/CNT cathode at 0.3 mV s^{-1} in in-situ Raman test.

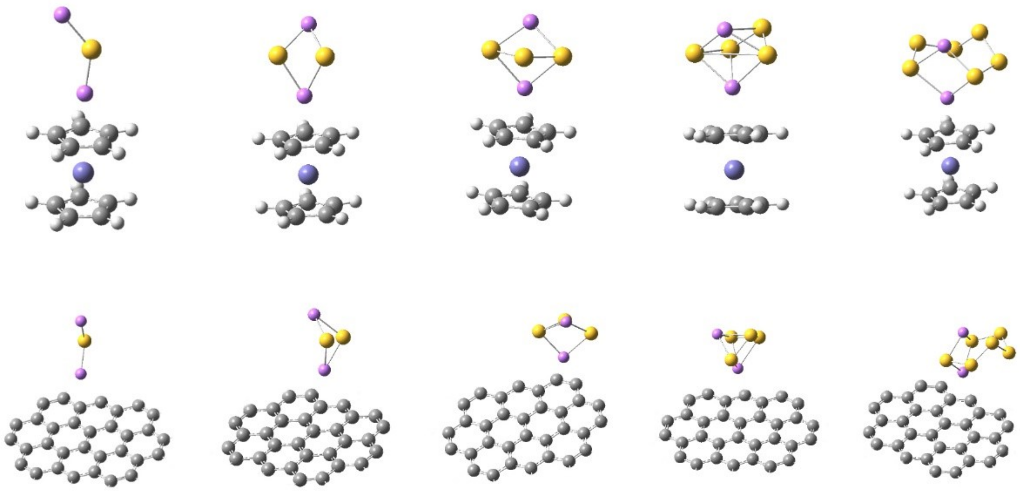

Fig. S6 The optimized structures of Li_2S, Li_2S_2, Li_2S_3, Li_2S_4, Li_2S_6 on the surface of ferrocene and CNT.

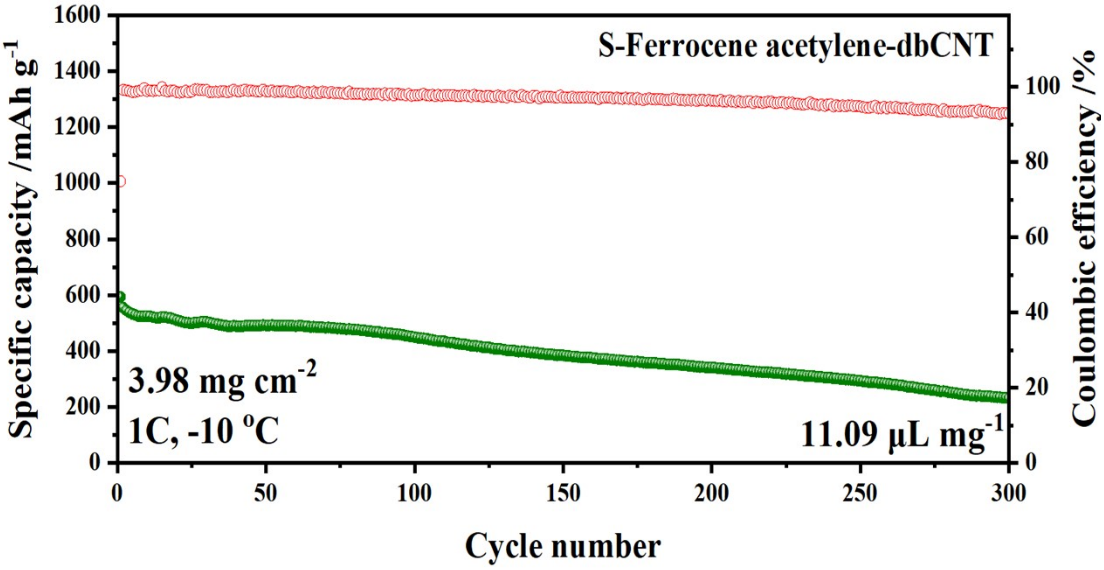

Fig. S7 Cycling performance of the cells with S-Ferrocene acetylene-dbCNT cathode at -10 ^{o}C.

Table S1. The sulfur content of S-Ferrocene acetylene-dbCNT, S-Ferrocene acetylene/CNT, S@Ferrocene/CNT and S@CNT via elemental analysis.

Name	Weight /mg	Methode	N /wt%	C /wt%	H /wt%	S /wt%	Average S /wt%
S-Ferrocene acetylene-dbCNT-1	3.136	5mg standard	---	32.270	0.880	60.756	61.560
S-Ferrocene acetylene-dbCNT-2	2.941	5mg standard	---	32.870	0.904	62.363	
S-Ferrocene acetylene/CNT-1	3.130	5mg standard	---	33.830	0.856	60.344	61.244
S-Ferrocene acetylene/CNT-2	3.020	5mg standard	---	32.590	0.842	62.143	
S@Ferrocene/CNT-1	3.182	5mg standard	---	32.440	1.059	63.647	63.561
S@Ferrocene/CNT-2	3.201	5mg standard	---	32.560	1.050	63.474	
S@CNT-1	3.096	5mg standard	---	39.910	---	62.698	62.723
S@CNT-2	3.035	5mg standard	---	40.200	---	62.748	

Table S2. The fitted impedance parameters of batteries based on S-Ferrocene acetylene-dbCNT, S-Ferrocene acetylene/CNT, S@Ferrocene/CNT, S@CNT.

Samples	R_s (Ω)	R_{ct} (Ω)
S-Ferrocene acetylene-dbCNT	3.36	24.91
S-Ferrocene acetylene/CNT	3.08	48.79
S@Ferrocene/CNT	2.45	87.21
S@CNT	5.59	144.26

Table S3. The lithium-ion diffusion coefficient for the cell with S-Ferrocene acetylene-dbCNT, S-Ferrocene acetylene/CNT, S@Ferrocene/CNT, S@CNT cathodes.

Samples	***C1*** ($\times 10^9$ cm^2 s^{-1})	***C2*** ($\times 10^9$ cm^2 s^{-1})	***A*** ($\times 10^9$ cm^2 s^{-1})
S-Ferrocene acetylene-dbCNT	114	373	410
S-Ferrocene acetylene/CNT	41.5	110.7	48.3
S@Ferrocene/CNT	34.4	53.2	48.9
S@CNT	5.31	9.58	7.6

Table S4. Comparison of the electrochemical performance of the reported covalently interlinked cathode for lithium-sulfur batteries. (1C=1675 mA g^{-1})

Cathode materials	Discharge current	Maximum Capacity (mAh g^{-1})	Sulfur loading (mg cm^{-2})	Capacity retention (Cycle Numbers)	Reference
S-Ferrocene acetylene-dbCNT	**0.5C**	**925**	**2.0**	**93.79% (400)**	**This work**
	1 C (14.96 mA cm^{-2})	**5.38 mAh cm^{-2}**	**8.93**	**81.97% (400)**	
	1 C，0 ℃	**685**	**2.0**	**75.54% (600)**	
SC@A	**0.5C**	**~1000**	**1.0**	**87% (200)**	**(1)**
SVE(1:9)	**0.5C**	**783**	**1-1.5**	**88.8% (400)**	**(2)**
TSP/CNT	**1C**	**728**	**0.6-0.8**	**54.4% (600)**	**(3)**
CNT@UiO-66-V-S	**0.2C**	**4.25 mAh cm^{-2}**	**5.6**	**91.76% (100)**	**(4)**
BTTPs	**0.1C**	**901**	**1.5-2**	**68.4% (120)**	**(5)**
GPS	**0.1C**	**920**	**1.15**	**76.08% (100)**	**(6)**
PTSeS/CG-CNT	**0.5C**	**591**	**1.0**	**62% (300)**	**(7)**

If not otherwise specified, the above batteries are tested at 30 ^{o}C.

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