Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Confinement of the Polysulfides within the Bi-functional Metal-Organic Framework for High Performance Lithium-Sulfur battery

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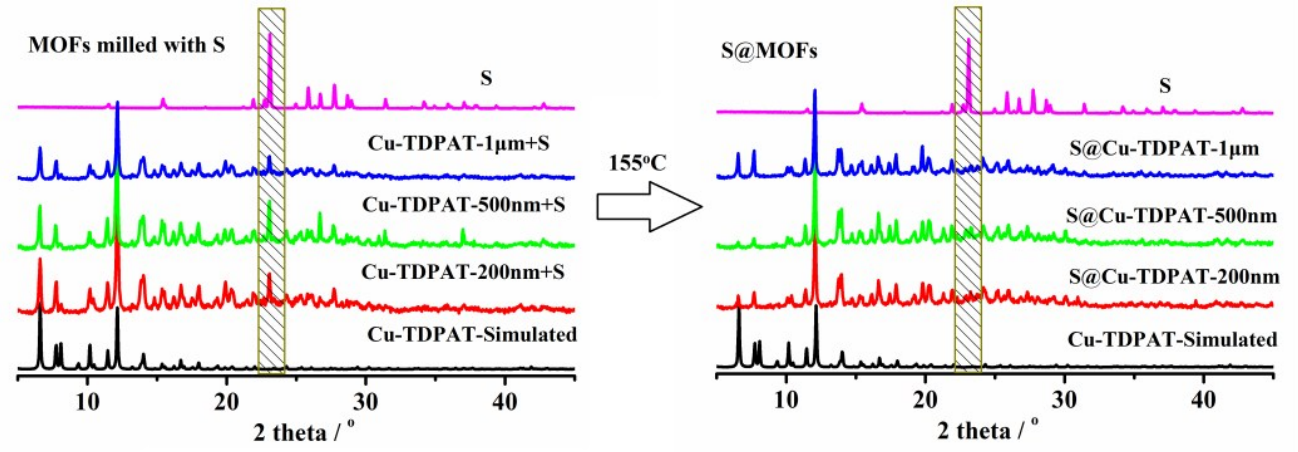

Figure **S1**. PXRD patterns of sulfur and Cu-TDPAT after ground (left) and after heated at 155°C (right).

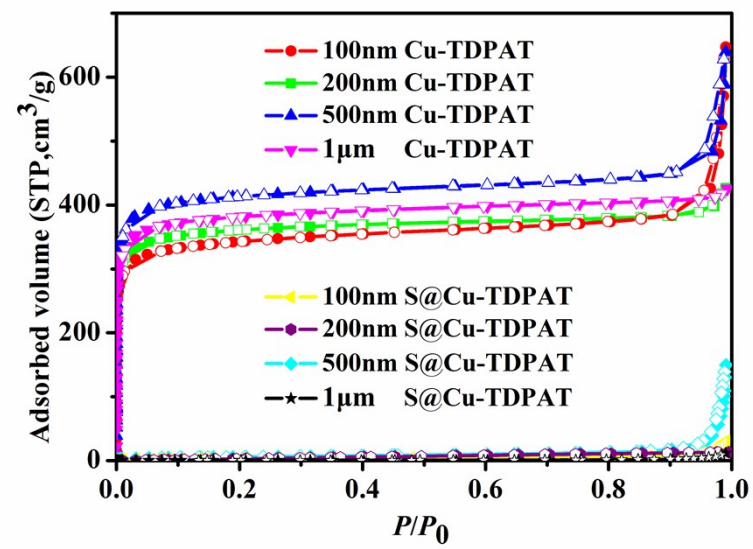

Figure **S2**. Adsorption isotherms of different size of nano Cu-TDPAT and S@Cu-TDPAT.

Table **S1**. Pore characterization results given by nitrogen adsorption measurement at 77K and the calculated sulfur contents in the composites.

	S_{BET}(m^2/g)[a]	pore size (nm)	V(cm^3/g)[b]	S/MOF(g/g)[c]	S content (%)[d]
100nm	1473	1.7645	0.55	1.001	50.0
200nm	1532	1.8662	0.62	1.128	53.0
500nm	1618	1.7766	0.63	1.146	53.4
1μm	1564	1.6832	0.61	1.110	52.6

[a]Fitting range : 0.005< p/p_0<0.05

[b]Calculated based on the adsorption volumes at p/p_0=0.05

[c]S/MOF=(density of molten sulfur, 1.82g/cm^3) × (pore volume at p/p_0=0.05)

[d]The largest amount of sulfur loading in the cage.

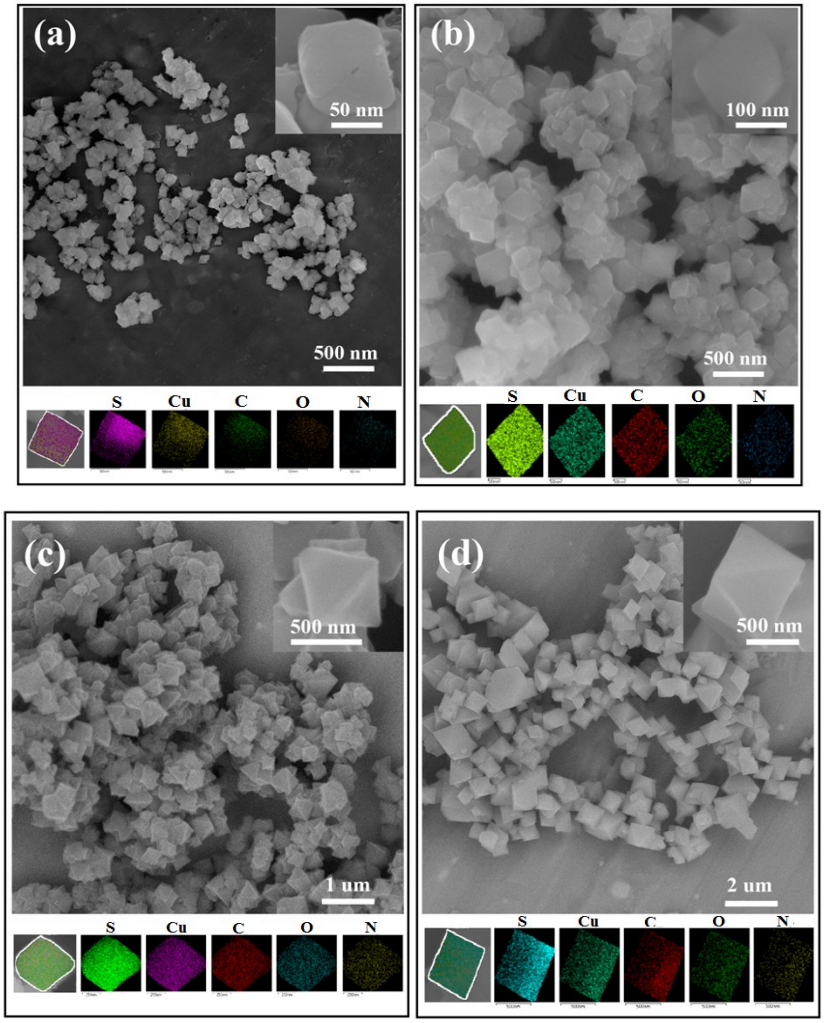

Figure **S3**. SEM and EDS mapping of S@Cu-TDPAT with different size (a) ~100nm; (b) ~200nm; (c) ~500nm; (d) ~1μm S@Cu-TDPAT.

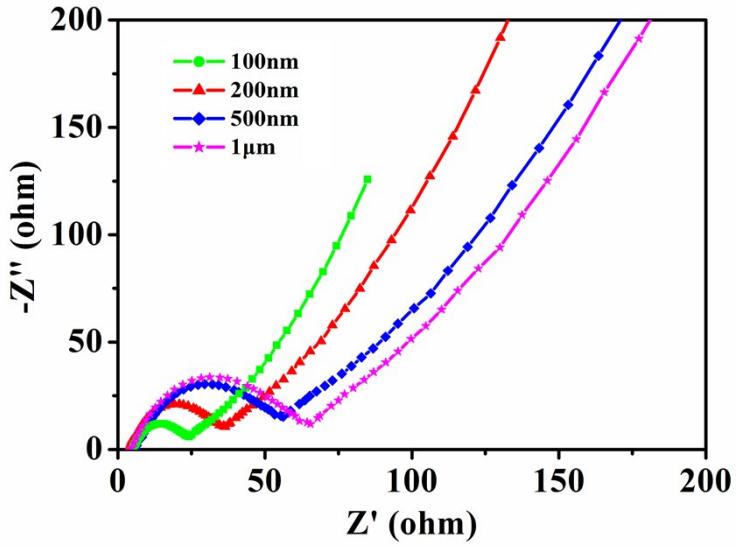

Figure **S4**. EIS plots of the S@Cu-TDPAT composite cathodes with different size before cycles.

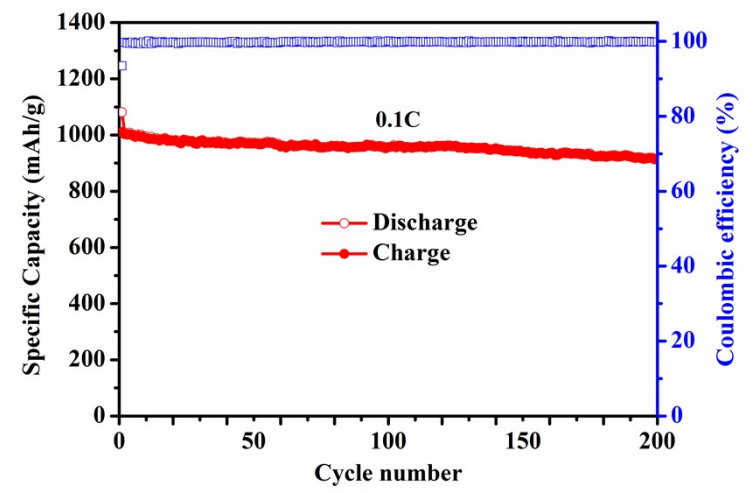

Figure **S5**. Cycling stability of S@Cu-TDPAT-100nm cathode at 0.1 C for 200 cycles.

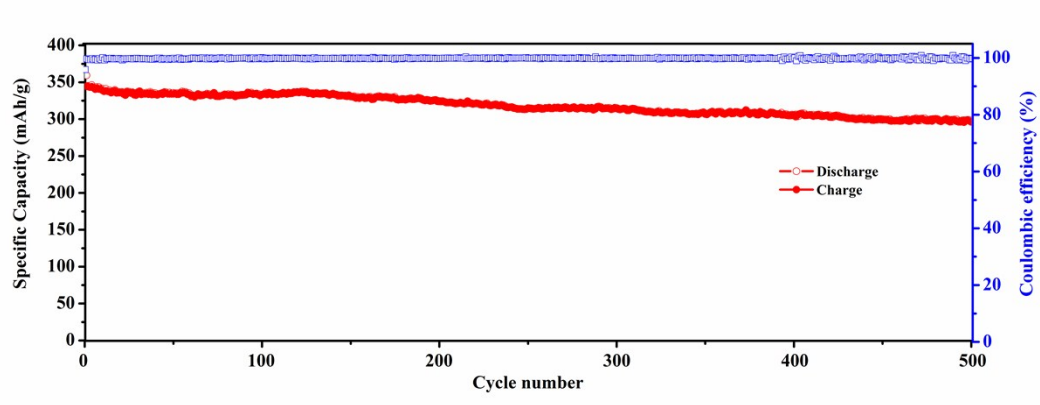

Figure **S6**. Cycling stability of S@Cu-TDPAT-100nm cathode at 1 C for 500 cycles (the capacity calculation based on the whole electrode including binder and electrolyte).

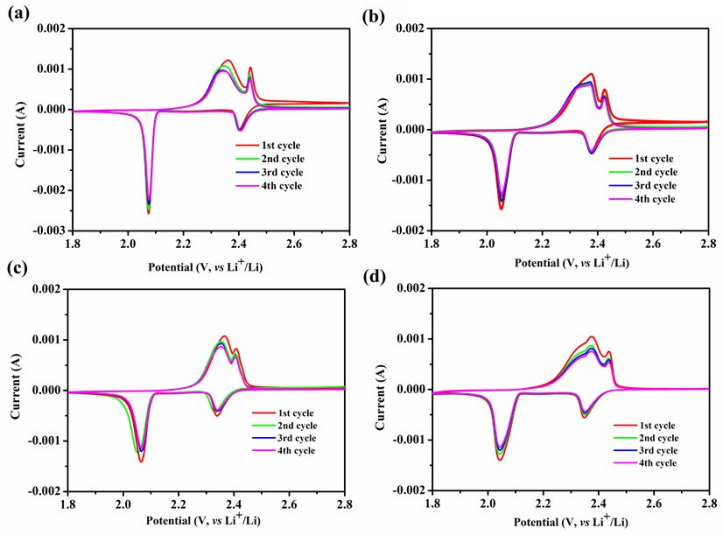

Figure **S7**. The cyclic voltammetry curves of S@Cu-TDPAT composites with different particle sizes: (a) 100nm; (b) 200nm; (c) 500nm; (d) 1μm.

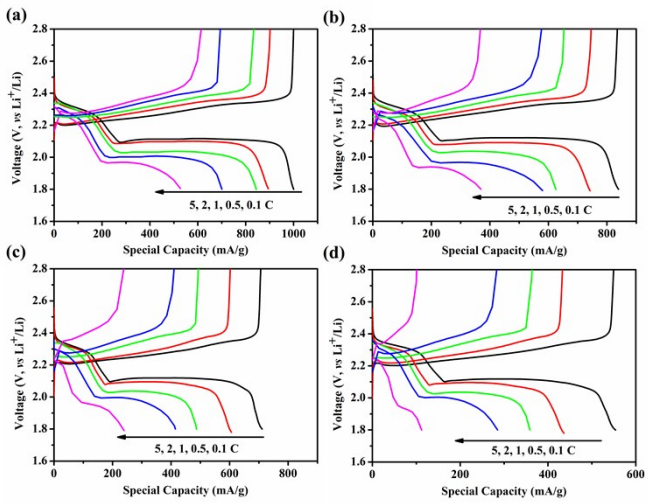

Figure **S8**. The galvanostatic discharge/charge profiles at different current rates of S@Cu-TDPAT with different size: (a) 100nm; (b) 200nm; (c) 500nm; (d) 1μm.

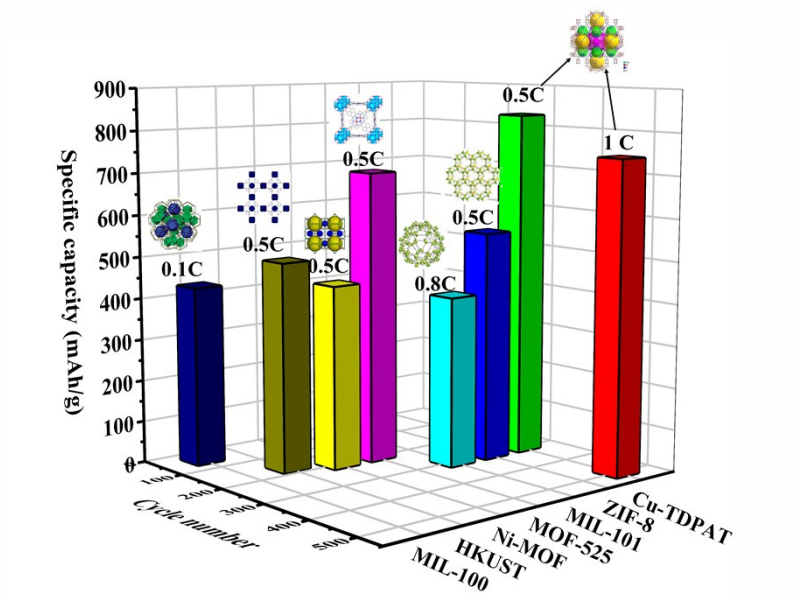

Figure **S9**. Comparison of the cycle performance of the reported partial sulfur/MOFs composite cathode materials.

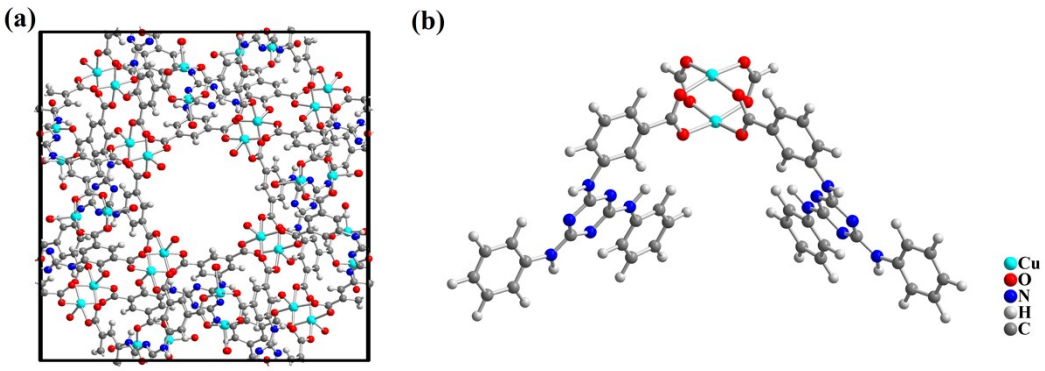

Figure **S10**. DFT optimized adsorption configuration. (a) Cu-TDPAT crystal cell containing 960 atoms. (b) a segment containing 104 atoms of $Cu_2(TDPAT)_2$.

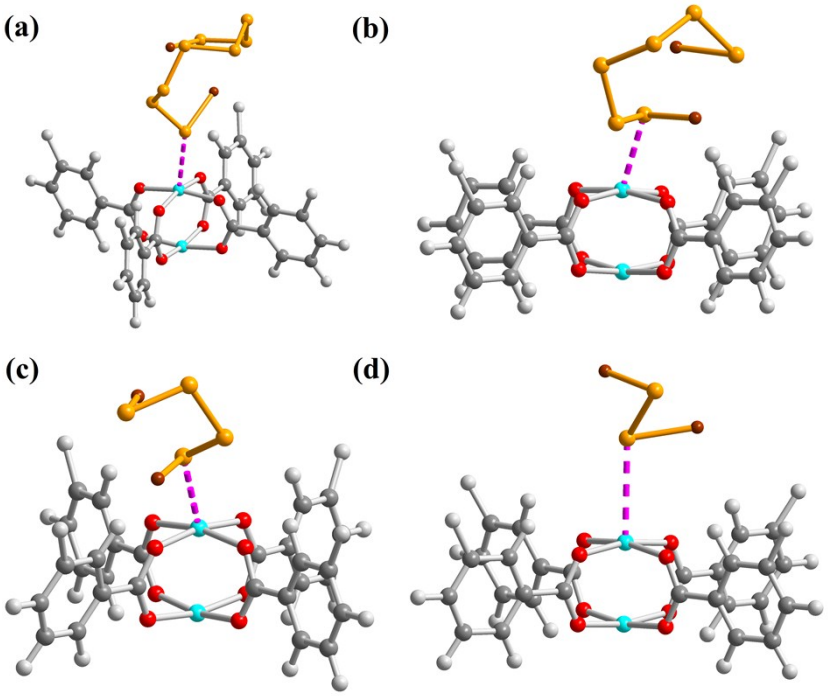

Figure **S11**. The interactions between polysulfide anions and Cu-TDPAT in the cage A. (a) Cu-TDPAT and Li_2S_8; (b) Cu-TDPAT and Li_2S_6; (c) Cu-TDPAT and Li_2S_4; (d) Cu-TDPAT and Li_2S_2.

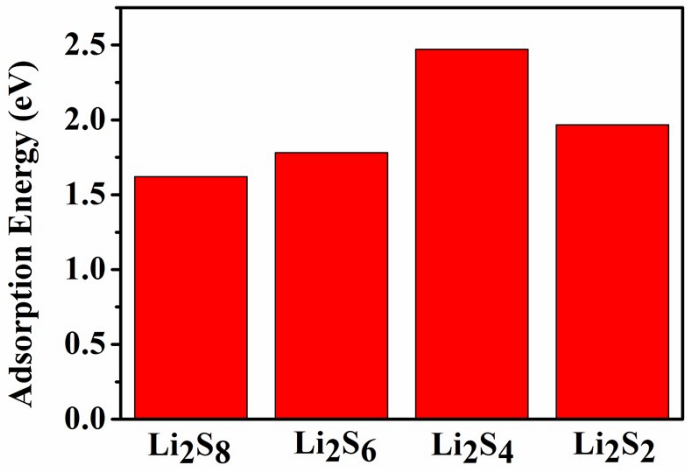

Figure **S12**. Calculated adsorption energy between Li_2S_x and $Cu_2(TDPAT)_2$.

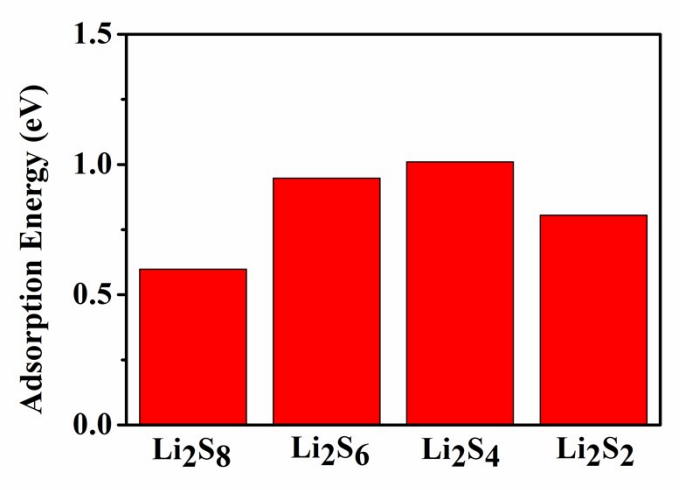

Figure **S13**. Calculated adsorption energy between Li_2S_x and Cu-TDPAT in the cage A.

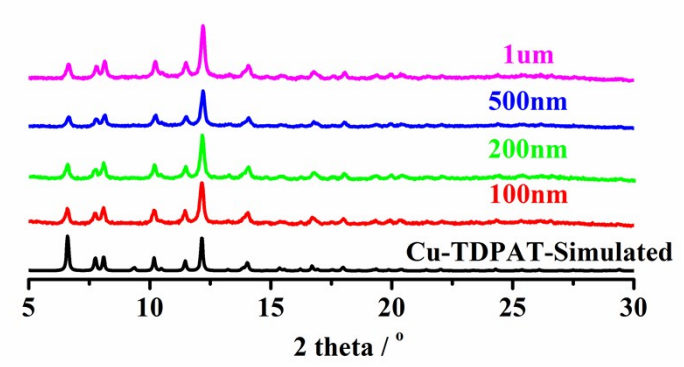

Figure **S14**. PXRD patterns of S@Cu-TDPAT after cycling at 0.5C.