

Supplementary Information for:

Improving electrochemical stability of lithium-sulfur battery with a conductive polymer coated-sulfur cathode

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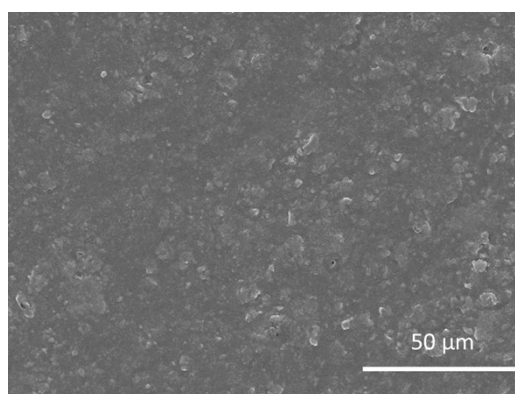


Fig. S1 SEM images of PEDOT:PSS-coated S cathode.

Assumptions of calculating energy density:

1. For the purpose of simplicity, only the mass and volume of active material, carbon and binder were considered.
2. All carbons have same density.
3. Lithium utilization is 90%.
4. $V_T = V_{\text{active}} + V_{\text{cb}} + V_{\text{binder}}$.
(V_T : total volume; V_{active} : volume of active material; V_{cb} : volume of carbon black; V_{binder} : volume of binder).
5. Carbon black and binder contribute no capacity.

Some parameters used:

Density: Lithium 0.534 g cm^{-3}

Carbon black 0.2 g cm^{-3}

SBR: 1.04 g cm^{-3}

CMC: 0.6 g cm^{-3}

PVDF: 1.77 g cm^{-3}

Sulfur: 2.07 g cm^{-3}

PEDOT:PSS: 1.011 g cm^{-3}

LiCoO₂: 5.1 g cm^{-3}

Graphite: 2.2 g cm^{-3}

Capacity for lithium-ion cell:

LiCoO₂: 150 mAh g^{-1}

Graphite: 350 mAh g^{-1}

Electrode mass ratio for lithium-ion cell:

LiCoO₂/CB/binder: 94/2/4

Graphite/CB/PVDF: 94/2/4

Average voltage for lithium-ion cell: $V_a = 3.7 \text{ V}$

Capacity and electrode mass ratio for Li-S cell: see the main text

Average voltage for Li/pristine S cell: $V_a = 2.1 \text{ V}$

A Average voltage for Li/P:P coated S cell: $V_a = 2.05 \text{ V}$

Method:

1. $1/C_{\text{tg}} = 1/C_{\text{ag}} + 1/C_{\text{cg}}$

(C_{tg} : total gravimetric capacity; C_{ag} : anode gravimetric capacity; C_{cg} : cathode gravimetric capacity)

$$2. \quad E_{\text{g}} = C_{\text{tg}} * V_{\text{a}}$$

(E_{g} : gravimetric energy density; C_{tg} : total gravimetric capacity; V_{a} : average voltage of a cell)

$$3. \quad 1/C_{\text{tv}} = 1/C_{\text{av}} + 1/C_{\text{cv}}$$

(C_{tv} : total volumetric capacity; C_{av} : anode volumetric capacity; C_{cv} : cathode volumetric capacity)

$$4. \quad E_{\text{v}} = C_{\text{tv}} * V_{\text{a}}$$

(E_{v} : volumetric energy density; C_{tv} : total volumetric capacity; V_{a} : average voltage of a cell)

For the lithium–sulfur system, the fifth charge and discharge data were used as the stabilized capacity for the input parameters.

Output results:

See Figure 7 in main text

Table S1 comparison of energy density between
the PEDOT:PSS-coated sulfur cathode and some typical sulfur-based composite cathodes
M1: Mass specific capacity only based on sulfur (mAh g⁻¹)
M2: Sulfur content in the cathode
M3: Mass specific capacity based on the total cathode (mAh g⁻¹)
M4: Gravimetric energy density of the cathode (Wh kg⁻¹)

	P:P-coated S	R13	R35	R23	R24	R22	R36	R12	R19	R39	R40
M1	1072	1050	1075	950	998	1250	1005	976	980	1065	1120
M2	60%	59%	46%	32%	34%	53%	55%	70%	82%	65%	56%
M3	643	617	492	304	343	662	550	687	803	692	627
M4	1319	1234	1008	544	618	1324	1100	1374	1526	1453	1317