

# The LiTFSI/COFs Fiber as Separator Coating with Bifunction of Inhibition of Lithium Dendrite and Shuttle Effect for Li-SeS<sub>2</sub> Battery

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Li<sup>+</sup> transfer number was calculated according to the following formula:

$$t_+ = \frac{I_s(\Delta V - I_0 R^0)}{I_0(\Delta V - I_s R^s)} \quad (1)$$

In this formula,  $t_+$  represents the ion transfer number;  $I_s$  is the current magnitude when constant voltage polarization is stable; constant voltage polarization is stable;  $\Delta V$  is the applied voltage;  $R^s$  is the interface impedance after constant voltage polarization;  $I_0$  is the starting current of constant voltage polarization;  $R^0$  is the interface impedance before constant voltage polarization. The Li<sup>+</sup> diffusion coefficient is calculated from the data provided by cyclic voltammetry. The calculation formula is as follows:

$$I_p = 2.69 \times 10^5 n^{1.5} A D_{Li^+}^{0.5} c_{Li^+} v^{0.5} \quad (2)$$

$I_p$  is the peak current of the corresponding oxidation peak or reduction peak;  $n$  is the number of transferred electrons;  $A$  is the area of the positive electrode plate;  $D_{Li^+}$  is the diffusion coefficient of Li<sup>+</sup>;  $c_{Li^+}$  is the concentration of Li<sup>+</sup>; and  $v$  is the scanning speed.

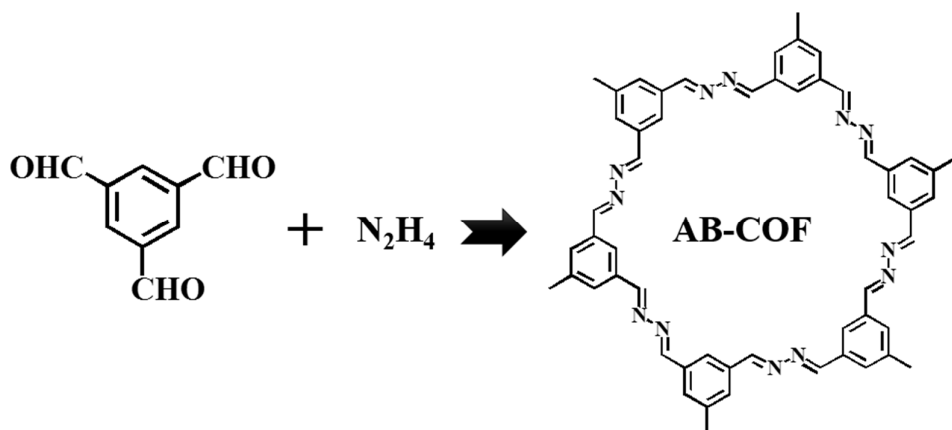


Figure S1. The structure of AB-COF.

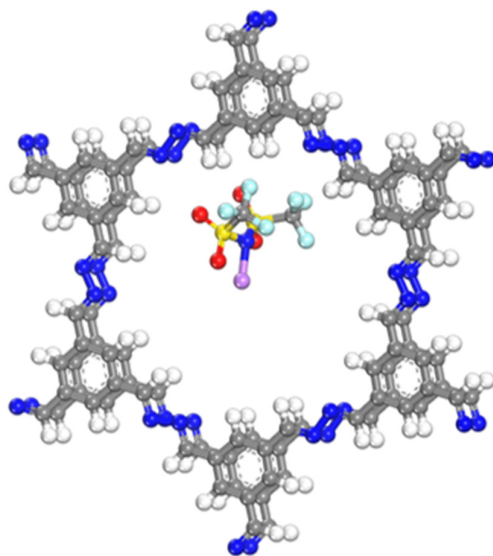


Figure S2. DFT calculation of LiTFSI/AB-COF.

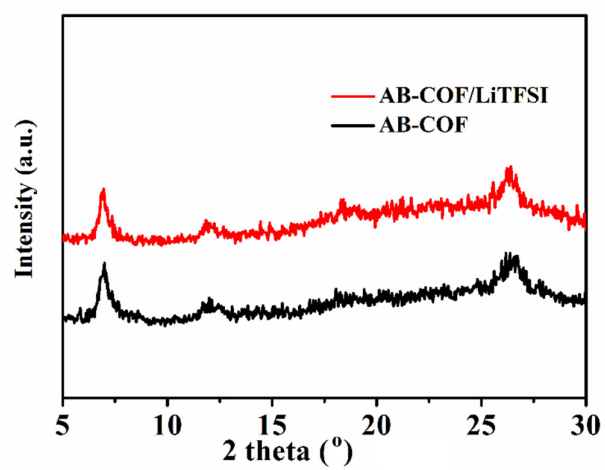
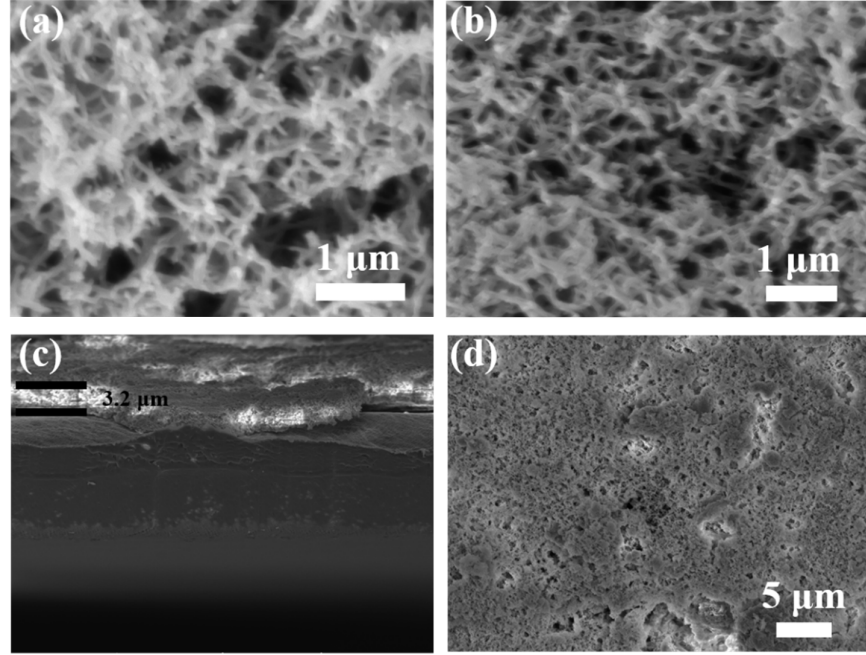
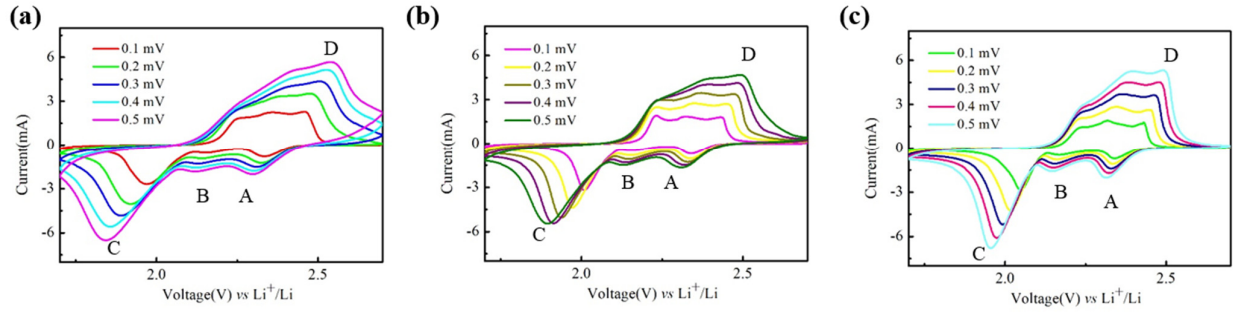


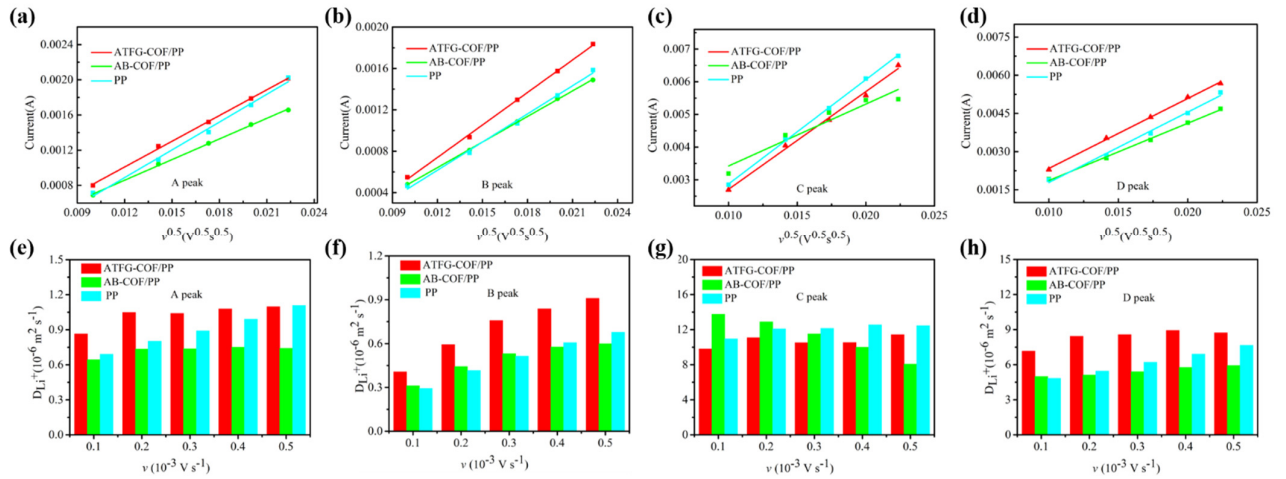
Figure S3. XRD spectrum of AB-COF and LiTFSI/AB-COF.



**Figure S4.** SEM pictures of (a) AB-COF and (b) LiTFSI/AB-COF. SEM of AB-COF/PP: (c) side view and (d) top view.

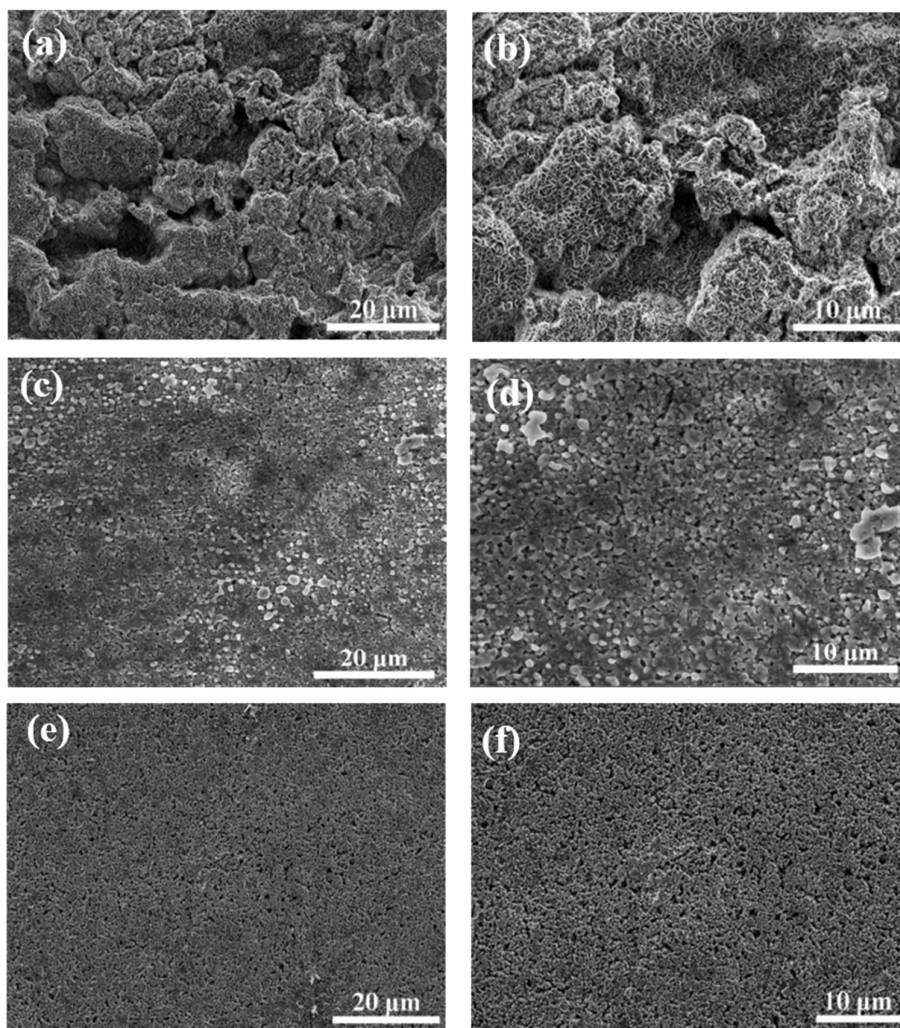


**Figure S5.** Cyclic voltammograms of Li-SeS<sub>2</sub> battery with (a) ATFG-COF/PP, (b) AB-COF/PP (c) PP separator at different sweep speeds.



**Figure S6.** Graph of CV peak current versus scan rate, (a) and (b) correspond to the conversion of SeS<sub>2</sub> to Li<sub>2</sub>Se<sub>n</sub> and Li<sub>2</sub>Se<sub>n</sub>, respectively; (c) correspond to the conversion of Li<sub>2</sub>Se<sub>n</sub> and Li<sub>2</sub>Se<sub>n</sub> to Li<sub>2</sub>S and

Li<sub>2</sub>Se, respectively; (d) Corresponding transformation of Li<sub>2</sub>S and Li<sub>2</sub>Se to SeS<sub>2</sub>. the relationship between Li<sup>+</sup> diffusion coefficient and sweep velocity V of Li-SeS<sub>2</sub> battery with ATFG-COF/PP, AB-COF/PP, PP at (e) A peak, (f) B peak, (g) C peak and (h) D peak.



**Figure S7.** SEM images of lithium metal anodes of the Li-SeS<sub>2</sub> cells with different separators after cycles. (a, b) PP, (c, d) AB-COF/PP, (e, f) ATFG-COF/PP separator.

**Table S1.** The comparison of the performance of the ATFG-COF/PP with the reported materials in Li-SeS<sub>2</sub> batteries.

Materials	Application	SeS <sub>2</sub> content	Current density (A g <sup>-1</sup> )	Cycle number	Specific Capacity (mAh/g)	Reference
ATFG-COF/PP separator	Separator	80 wt%	0.5C	200	509	This work
SAZ-AF Janus separator	Separator	80 wt%	1.1	200	446.4	[1]
CoS <sub>2</sub> @LRC/SeS <sub>2</sub>	cathode	70wt%	0.5	400	470	[2]
CMK-3/SeS <sub>2</sub> @PDA	cathode	70 wt%	2	500	350	[3]
TiN/GO	separator	70 wt%	1	500	511	[4]

## References

1. Song, C.-L.; Li, Z.-H.; Ma, L.-Y.; Li, M.-Z.; Huang, S.; Hong, X.-J.; Cai, Y.-P.; Lan, Y.-Q. Single-Atom Zinc and Anionic Framework as Janus Separator Coatings for Efficient Inhibition of Lithium Dendrites and Shuttle Effect. *ACS Nano* **2021**, *15*, 13436–13443.
2. Zhang, J.; Li, Z.; Lou, X.W. A Freestanding Selenium Disulfide Cathode Based on Cobalt Disulfide-Decorated Multichannel Carbon Fibers with Enhanced Lithium Storage Performance. *Angew. Chem. Int. Ed.* **2017**, *56*, 14107–14112.
3. Li, Z.; Zhang, J.; Wu, H.B.; Lou, X.W. An Improved Li-SeS<sub>2</sub> Battery with High Energy Density and Long Cycle Life. *Adv. Energy Mater.* **2017**, *7*, 1700281.
4. Zhang, Y.; Guo, Y.; Wang, B.; Wei, Y.; Jing, P.; Wu, H.; Dai, Z.; Wang, M.; Zhang, Y. An integrated hybrid interlayer for polysulfides/selenides regulation toward advanced Li-SeS<sub>2</sub> batteries. *Carbon* **2020**, *161*, 413–422.