

Supporting Information

Iodine doping induced activation of covalent organic framework cathodes for Li-ion batteries

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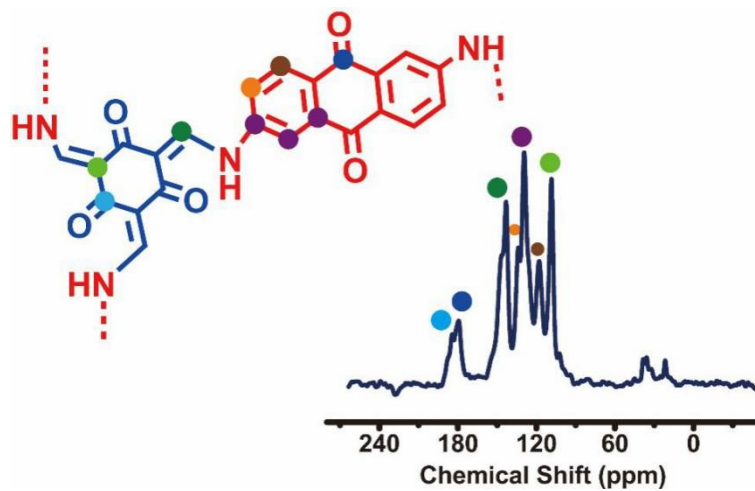
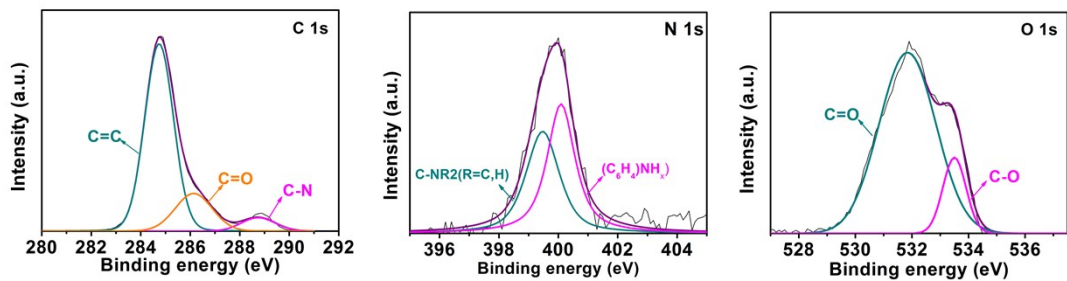


Figure S1. Solid-state ^{13}C NMR spectrum of COF. The corresponding carbons are labeled in the structural motif (inset).

COF



COF-I

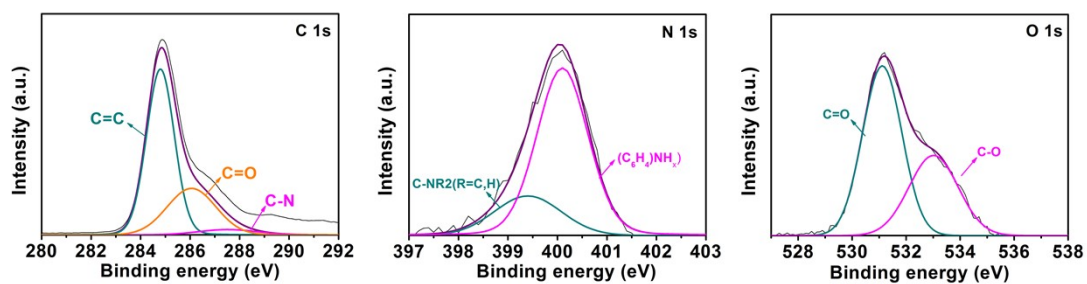


Figure S2. C 1s, N 1s, and O 1s high-resolution XPS spectra of COF and COF-I.

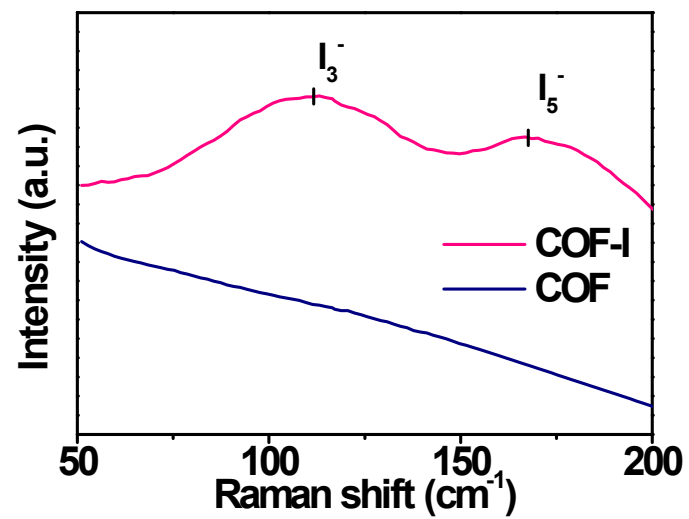


Figure S3. Raman spectra of COF and COF-I.

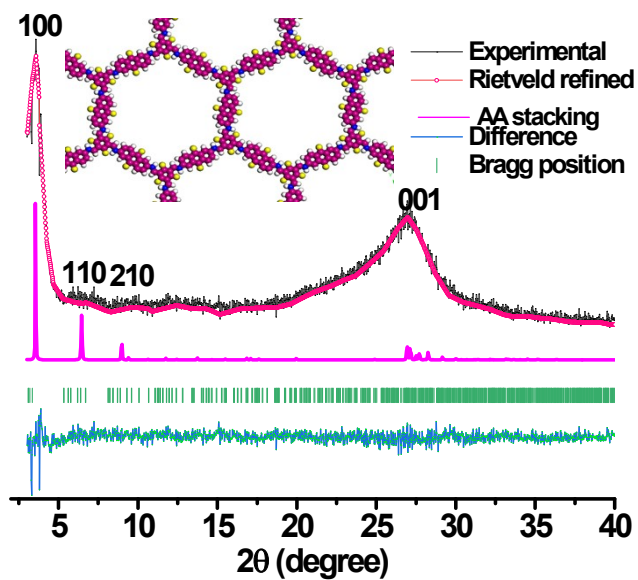
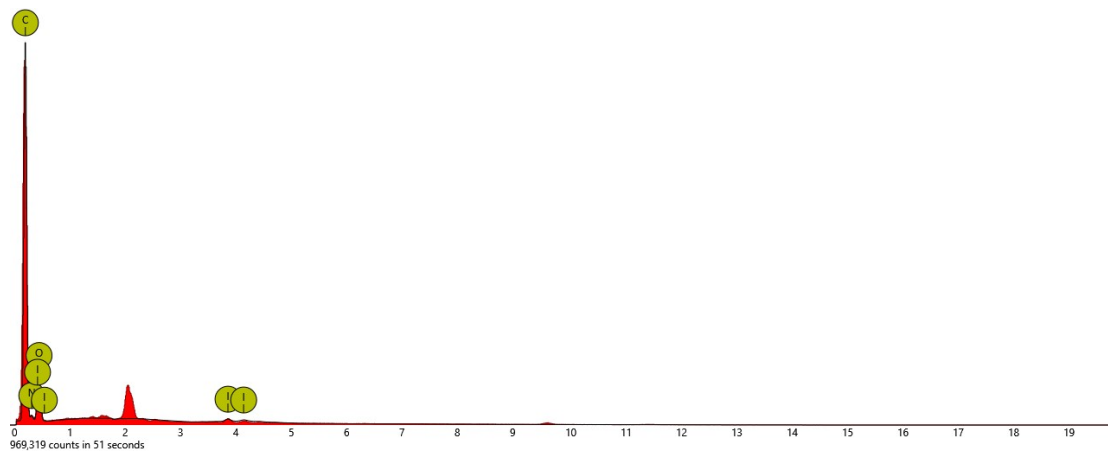


Figure S4. Experimental PXRD patterns, Pawley-refined patterns, simulated patterns, difference plots, Bragg positions for COF. The inset shows the simulated structure.



Weight percentage

C	64.58 %
O	22.60 %
N	10.91 %
I	1.92 %

Figure S5. Energy-dispersive spectroscopy of COF-I.

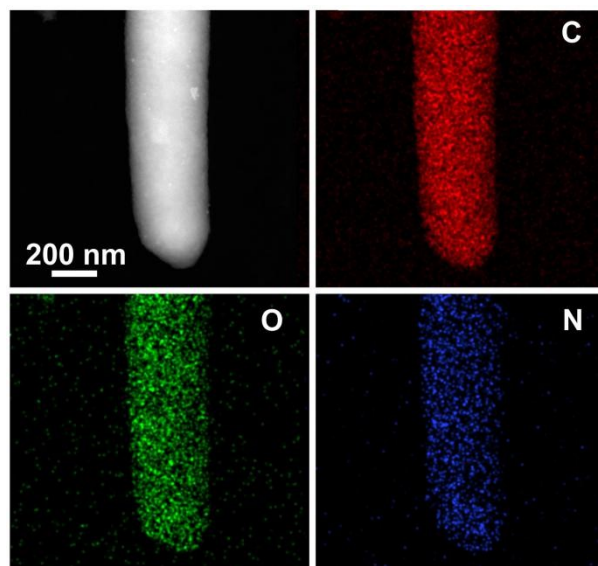


Figure S6. Energy-dispersive spectroscopy (EDS) elemental mapping images of C, N, O from the skeleton of COF. EDS images confirm the rodlike structure with a uniform distribution of C, N, O elements.

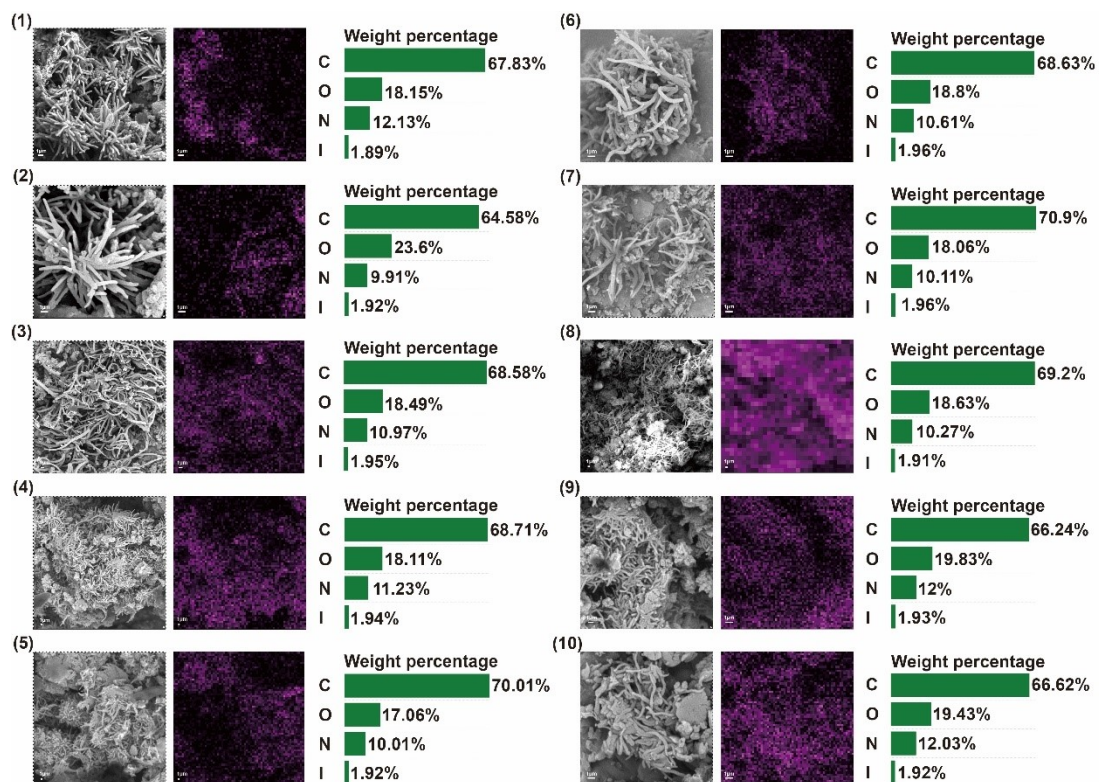


Figure S7. SEM images and the corresponding EDS for ten different batches of COF-I samples.

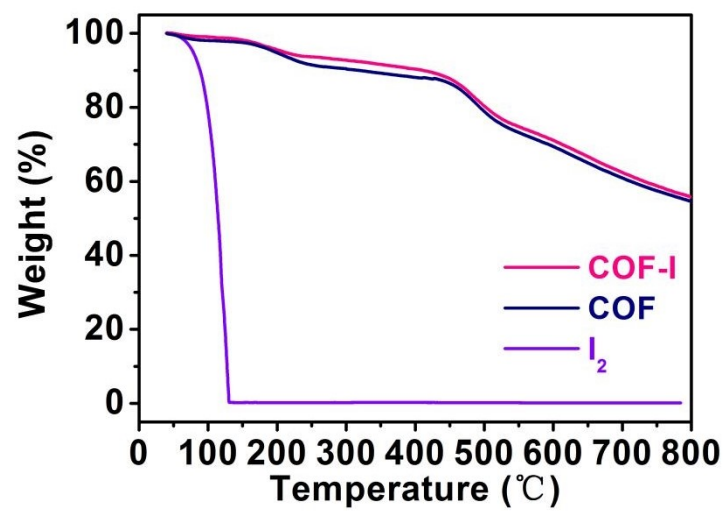


Figure S8. Thermogravimetric analysis curves of I₂, COF and COF-I.

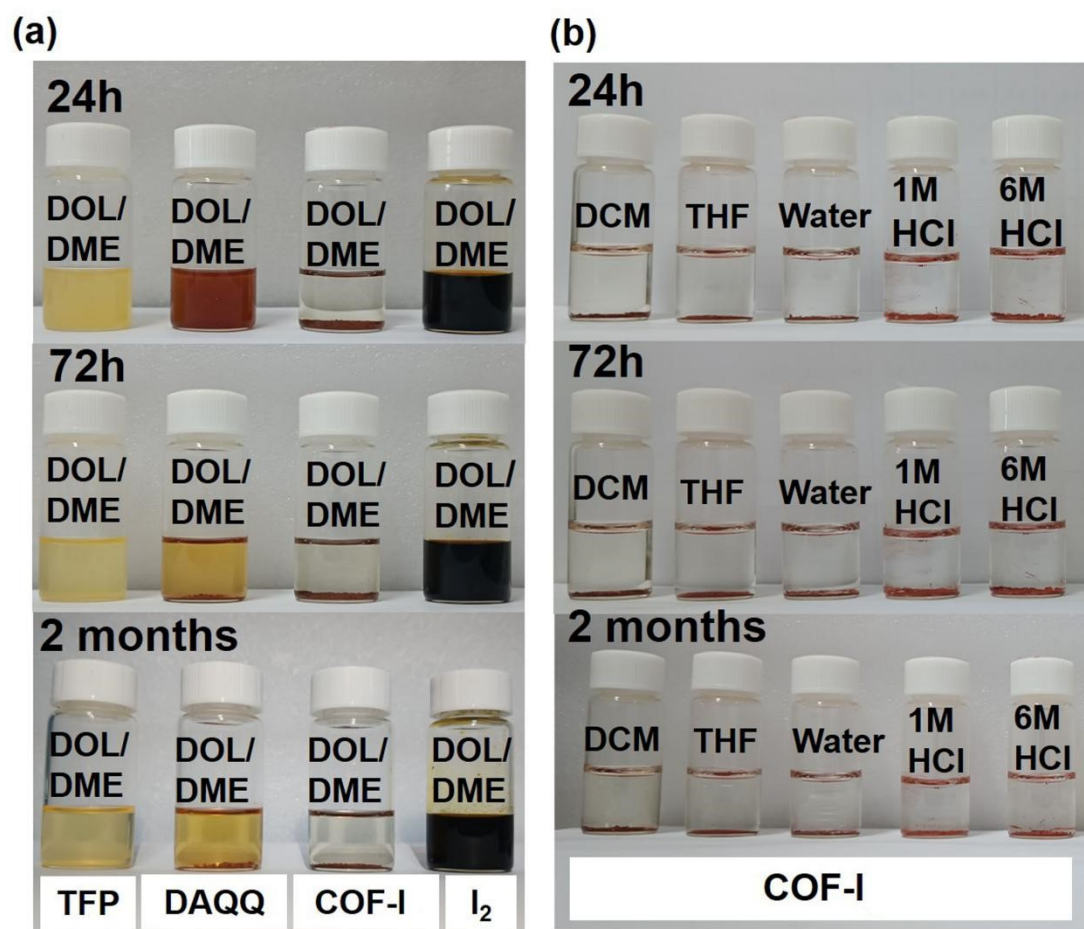


Figure S9. Chemical stability tests of COF-I in general solvents for 24h, 72h and 2 months.

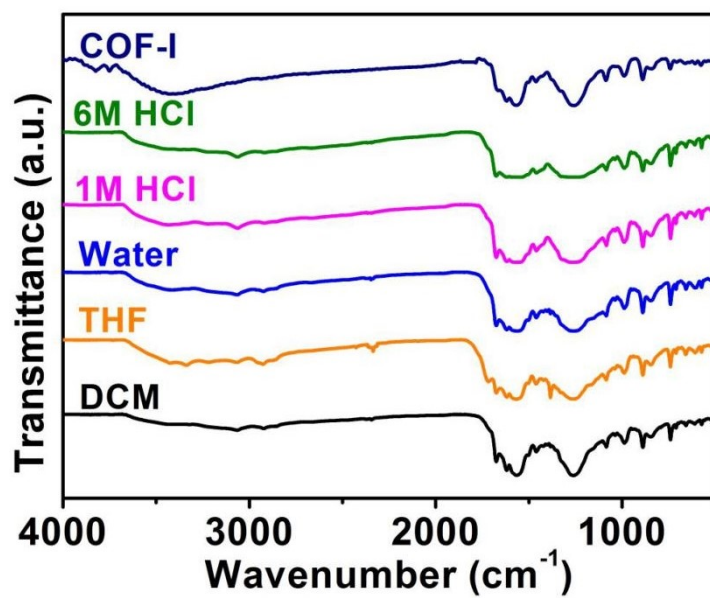


Figure S10. FT-IR spectra of COF-I after soaking in DCM, THF, water, 1M and 6 M HCl (aq.) for 24 hours.

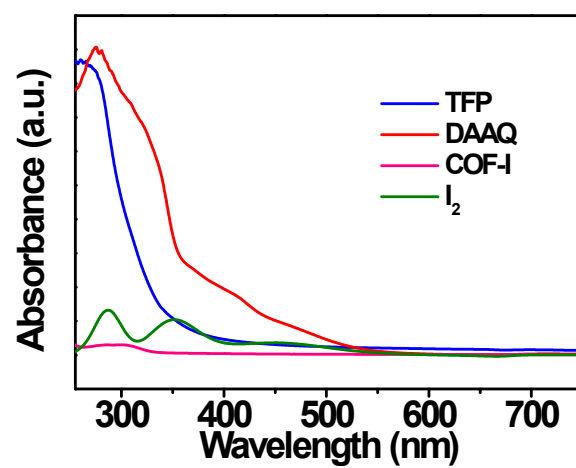


Figure S11. UV-vis absorption spectra of TFP, DAAQ, COF-I, I₂ after immersion treatments in 1,3-Dioxolane (DOL) / dimethoxyethane (DME) solvent for 2 months.

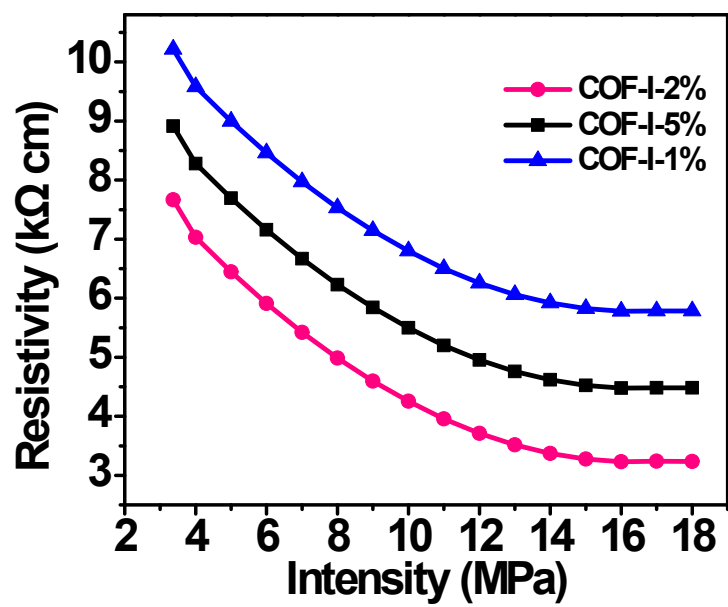


Figure S12. Relationship between pressure and resistivity for COF-I-1%, COF-I-2%, and COF-I-5%.

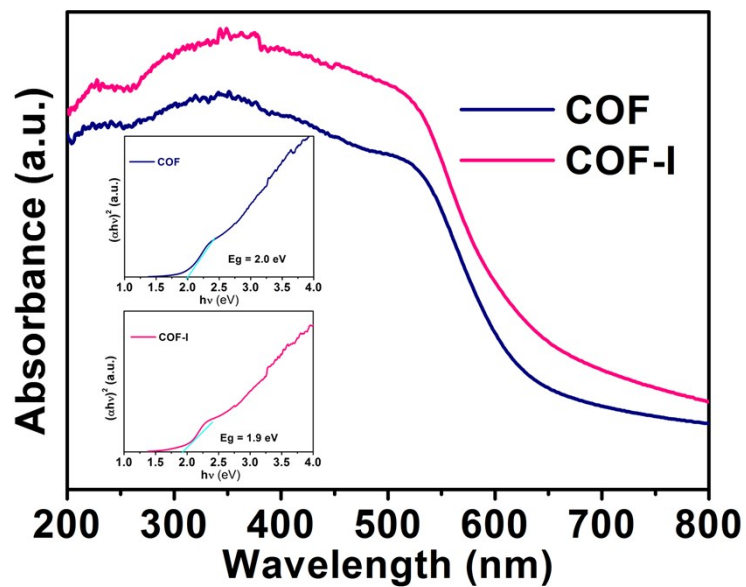


Figure S13. Solid-state UV-vis diffuse reflectance spectra for COF and COF-I. (inset) The corresponding K-M-transformed reflectance spectra.

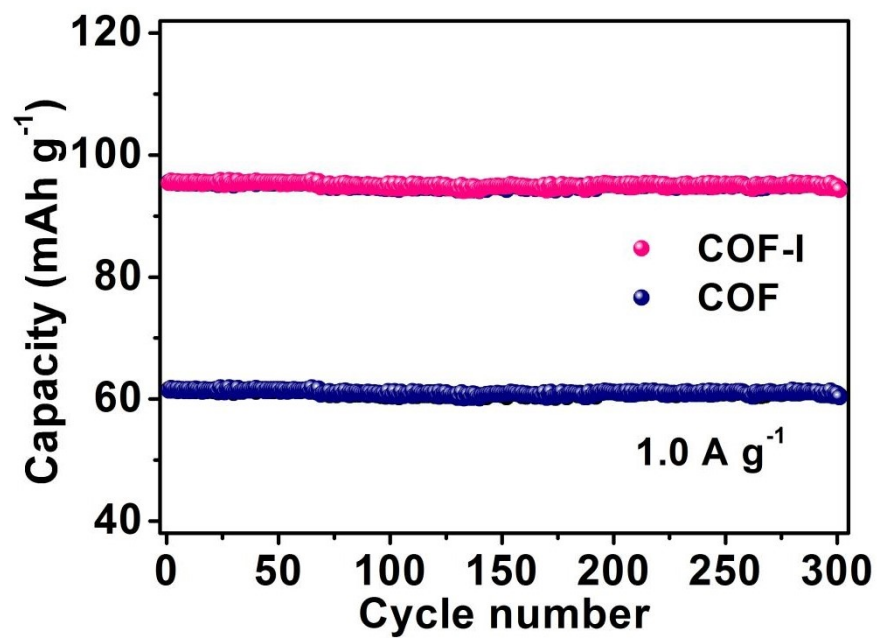


Figure S14. Cycling performances over 300 cycles at 1.0 A g⁻¹ for COF and COF-I.

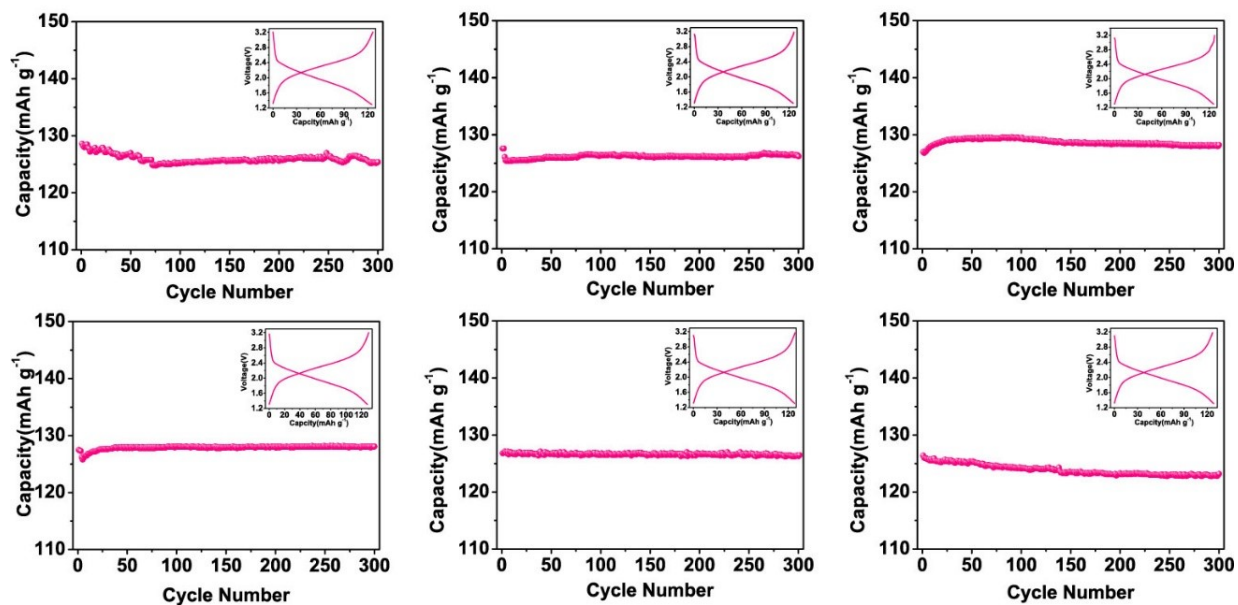


Figure S15. Cycling performances for six different batches of COF-I at 0.2 A g⁻¹.

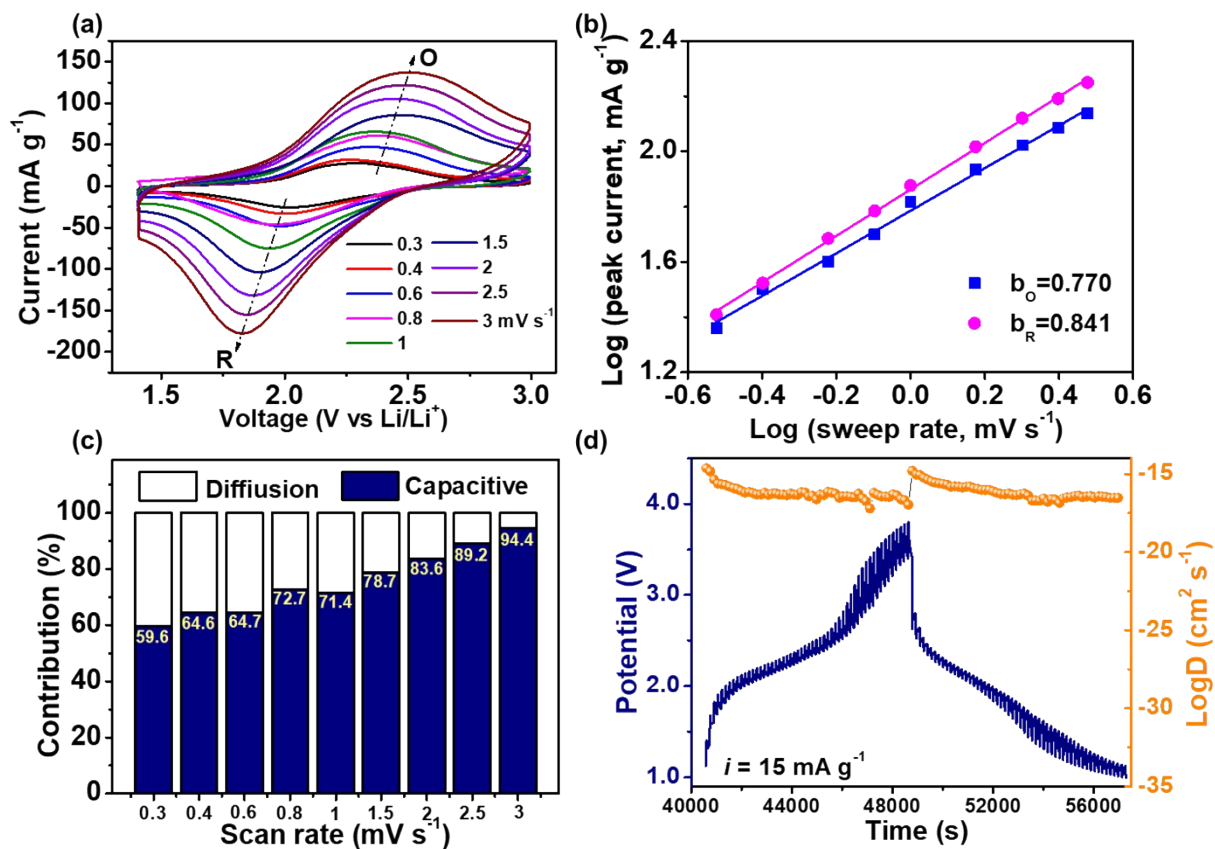


Figure S16. Kinetics analysis of COF. (a) CV curves obtained at different scan rates; (b) $\log(i)$ versus $\log(v)$ plots to determine the b values; (c) capacitive and diffusion contribution ratios to the total capacity at different scan rates; (d) GITT tests and corresponded ion diffusion coefficient of COF.

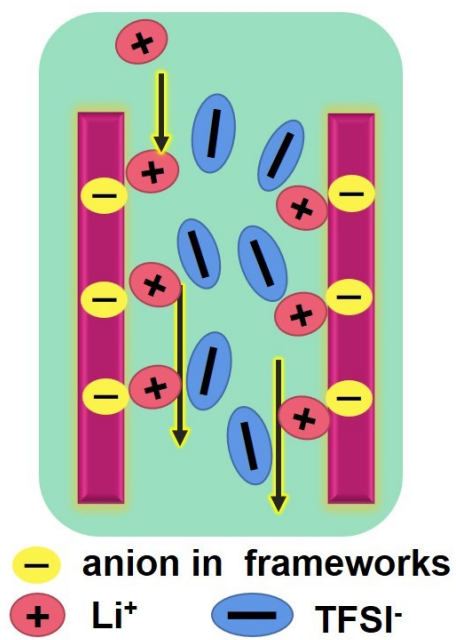


Figure S17. The diagram of Li⁺ transport in COF-I.

Table S1. A comparison of the electrical properties of some previously reported COF materials at room temperature.

	COFs	Carrier mobility (cm ² V ⁻¹ s ⁻¹)	Carrier mobility after iodine doping (cm ² V ⁻¹ s ⁻¹)	Conductivity (S m ⁻¹)	Conductivity after iodine doping (S m ⁻¹)	References
1	DAAQ-COF	8.36	11.05	1.63×10 ⁻⁴	2.28×10 ⁻³	This work□
2	NiPc-CoTAA	0.15	-	8.16×10 ⁻³	0.52	[S1]
3	COF-DC-8	8.10	-	2.51×10 ⁻³	2.51	[S2]
4	TTF-COF	-	-	1.20×10 ⁻⁴	0.28	[S3]
5	POR-COF	-	-	4.6×10 ⁻⁹	1.52×10 ⁻⁵	[S4]
6	WBDT	-	-	2.7×10 ⁻⁴	4.72×10 ⁻²	[S5]
7	ZnPc-pz	4.80	22	7.0×10 ⁻⁵	3.1×10 ⁻²	[S6]
8	CuPc-pz	0.90	7	3.3×10 ⁻⁵	1×10 ⁻²	
9	TTF-ph-COF	0.2	-	-	1.00×10 ⁻³	[S7]
10	sp ² c-COF	-	-	6.1×10 ⁻¹⁴	7.10×10 ⁻²	[S8]
11	TANG-COF	-	-	1.6×10 ⁻³	0.15	[S9]
12	3D p-POP	-	-	5×10 ⁻⁸	2.9×10 ⁻⁵	[S10]
13	BUCT-COF-4	1.97	2.62	5.75×10 ⁻⁶	2.79×10 ⁻⁴	[S11]

References

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