Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

A cobalt-based metal–organic framework and its derived material as sulfur hosts for aluminum-sulfur batteries with chemical anchoring effect

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Table S1. Calculated total energies of ZIF-67, ZIF-67-700, S_8, Al_2S_3, Al_2S_6, Al_2S_{12}, Al_2S_{18}, and the corresponding adsorption models.

	ZIF-67	ZIF-67-700	S_8	Al_2S_3	Al_2S_6	Al_2S_{12}	Al_2S_{18}
Total energy / eV	-66440.98	/	-86655.18	-45687.18	-78185.06	-143178.97	-208171.03
/	/	/	S_8@ZIF-67	Al_2S_3@ZIF-67	Al_2S_6@ZIF-67	Al_2S_{12}@ZIF-67	Al_2S_{18}@ZIF-67
Total energy / eV	/	-66504.36	-153097.53	-112128.47	-144627.38	-209620.32	-274612.50
/	/	/	S_8@ZIF-67-700	Al_2S_3@ZIF-67-700	Al_2S_6@ZIF-67-700	Al_2S_{12}@ZIF-67-700	Al_2S_{18}@ZIF-67-700
Total energy / eV	/	/	-153162.85	-112193.45	-144691.91	-209685.50	-274677.81

Table S2. Calculated binding energies and charge transfer of sulfur and intermediate polysulfides when adsorbing on ZIF-67 or ZIF-67-700.

	S_8	Al_2S_3	Al_2S_6	Al_2S_{12}	Al_2S_{18}
Binding energy on ZIF-67 / eV	-1.38	-0.31	-1.34	-0.37	-0.50
Binding energy on ZIF-67-700 / eV	-3.31	-1.91	-2.49	-2.17	-2.42
Charge transfer on ZIF-67 / *e*	-0.161	-0.131	-0.369	-0.227	-0.495
Charge transfer on ZIF-67-700 / *e*	-1.174	-0.703	-1.065	-1.060	-1.078

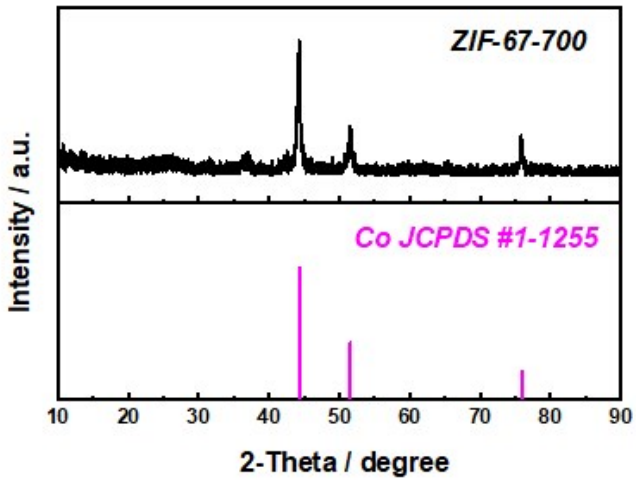

Figure S1 XRD patterns of ZIF-67-700 and metal cobalt (JCPDS #1-1255)

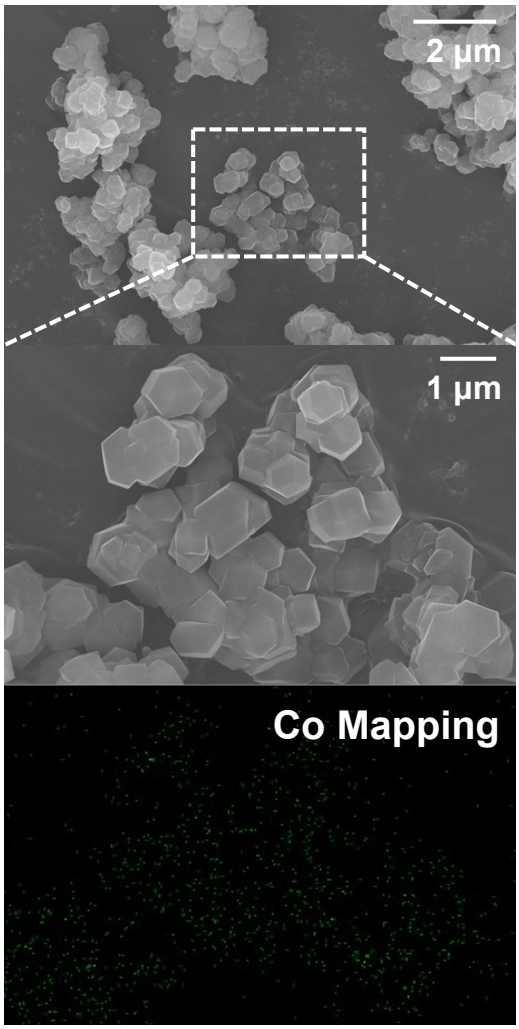

Figure S2 SEM and EDS images of ZIF-67 polyhedrons.

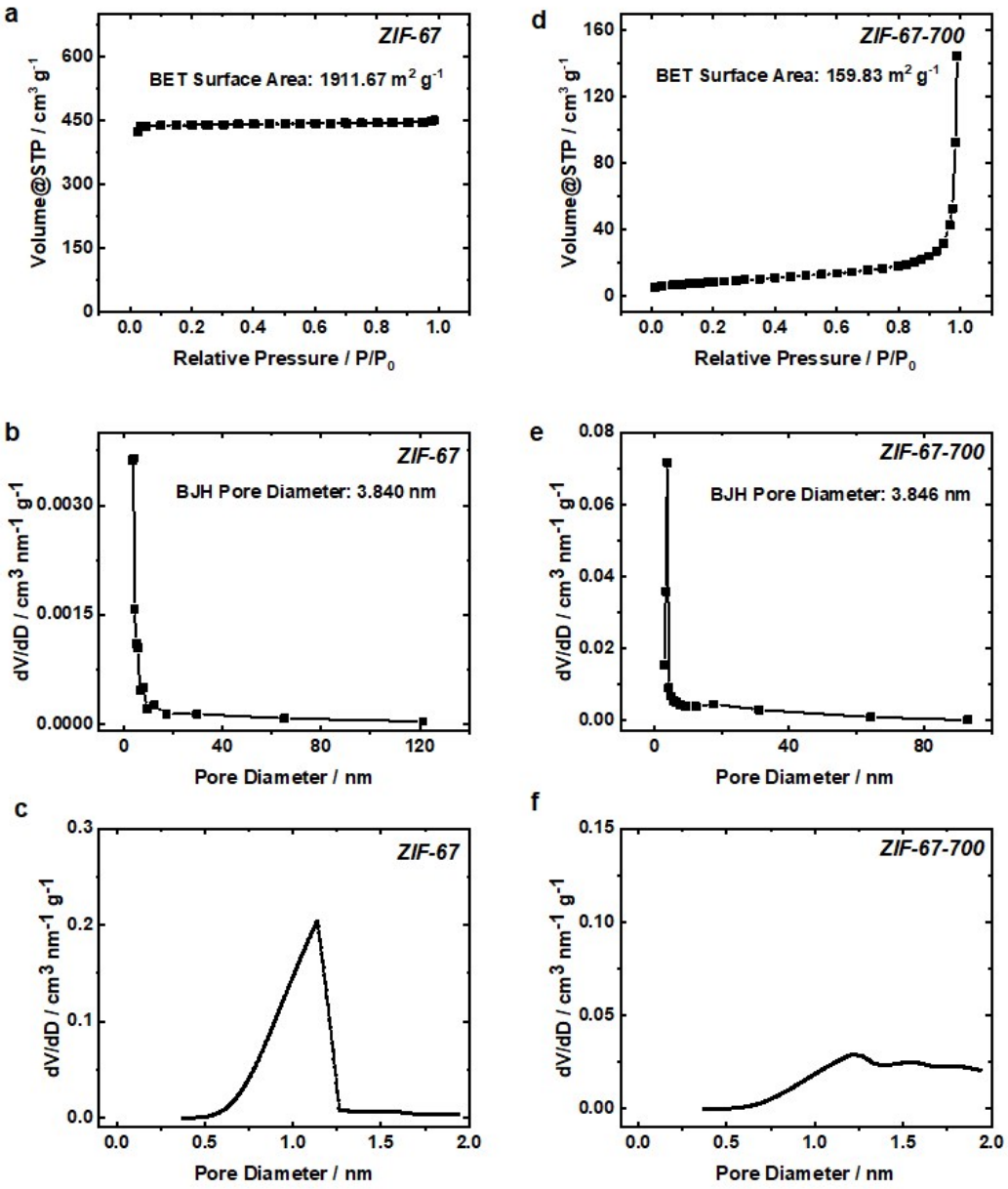

Figure S3 (a, d) N_2 adsorption/desorption isotherm plots, (b, e) mesoporous size distribution calculated via BJH method, (c, f) microporous size distribution via HK method for ZIF-67 and ZIF-67-700, respectively.

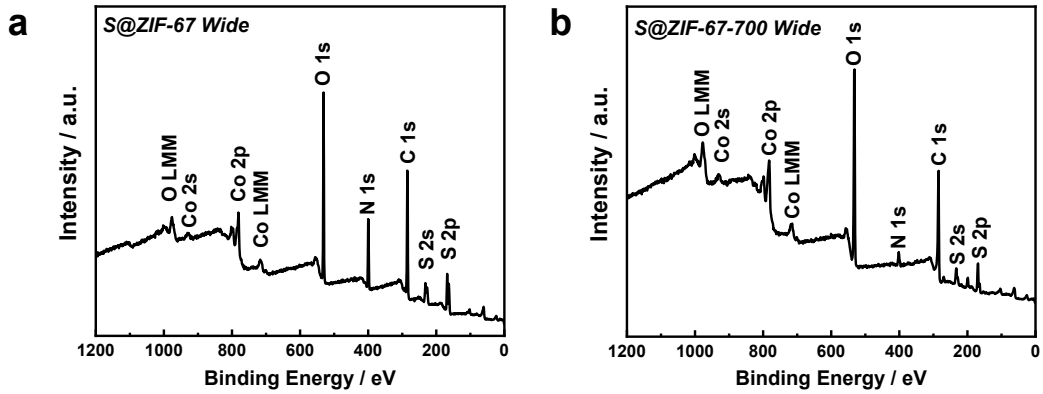

Figure S4 XPS wide spectra of (a) S@ZIF-67 and (b) S@ZIF-67-700.

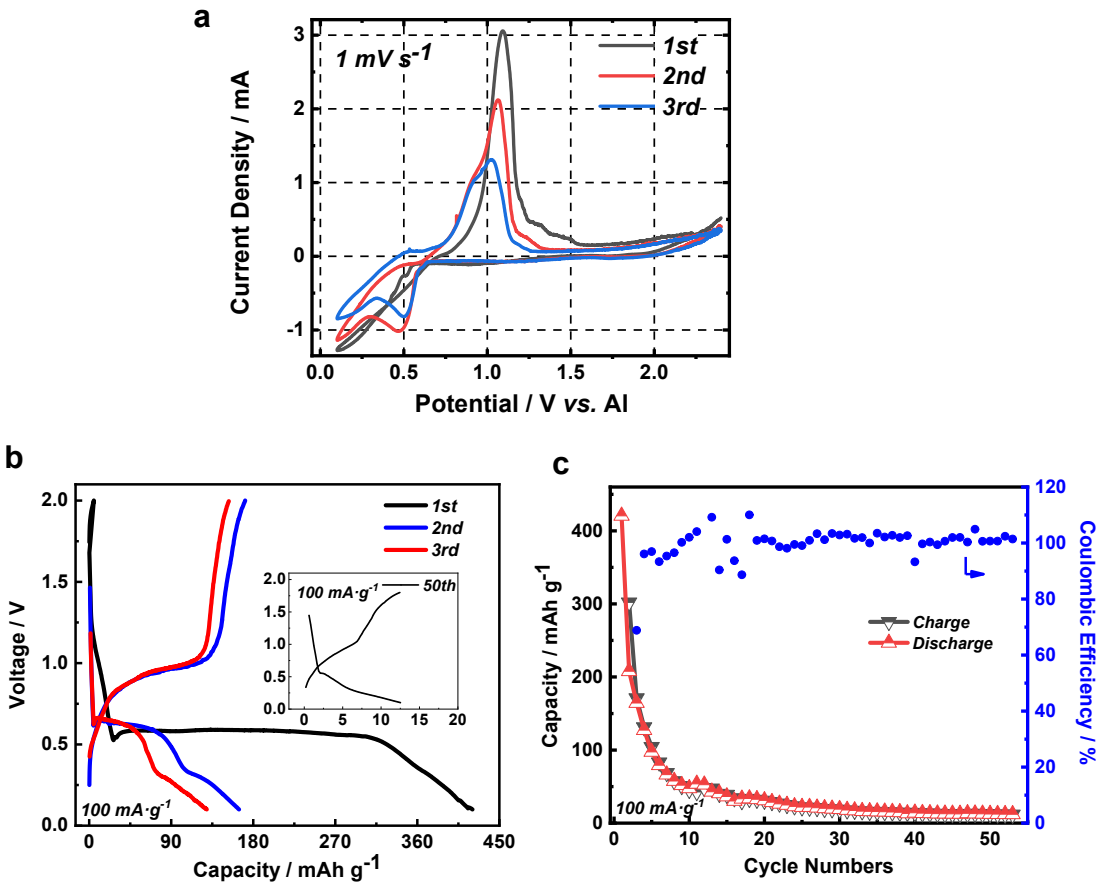

Figure S5 (a) CV curve, (b) Charge and discharge voltage profiles, (c) Cycling performance of ZIF-67.

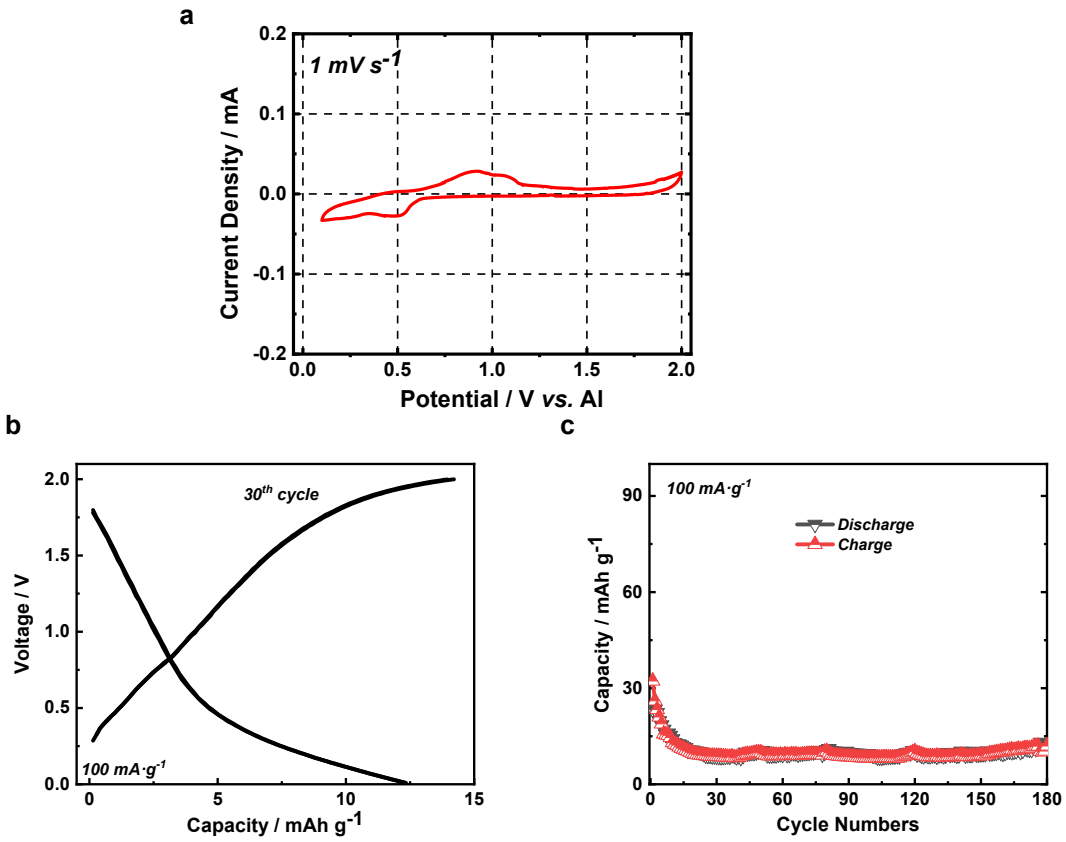

Figure S6 (a) CV curve, (b) Charge and discharge voltage profiles, (c) Cycling performance of ZIF-67-700.

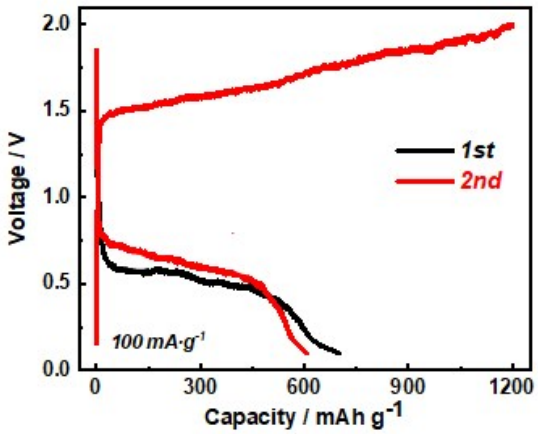

Figure S7 Charge/discharge voltage profile of S@ZIF-67-700 at a current density of 100 mA g^{-1}.

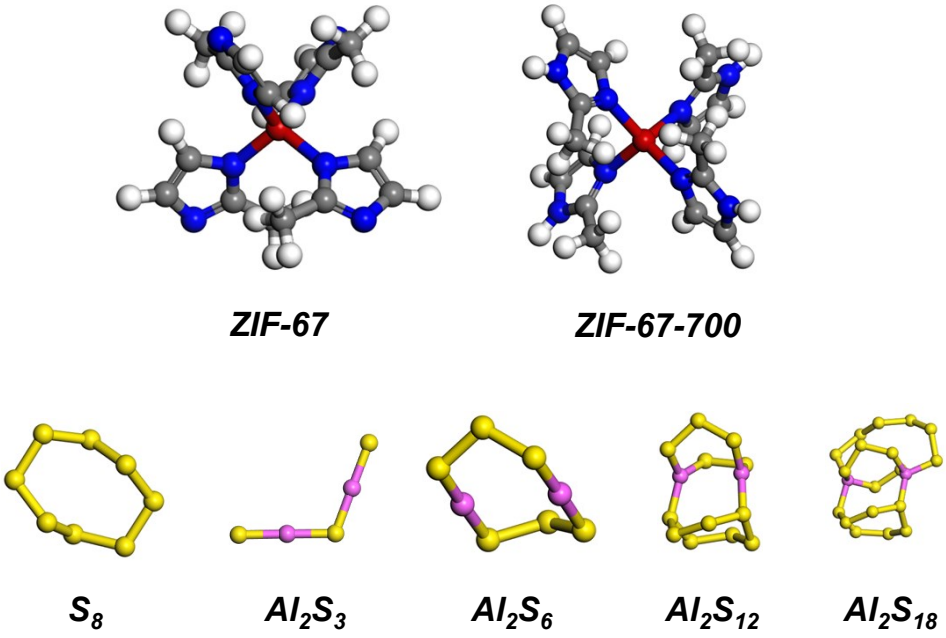

Figure S8 Relaxed structures of ZIF-67, ZIF-67-700, S_8, Al_2S_3, Al_2S_6, Al_2S_{12}, and Al_2S_{18}, respectively. Carbon, hydrogen, nitrogen, cobalt, sulfur, aluminum atoms were denoted using gray, white, blue, red, magenta, and yellow spheres, respectively.