Electronic Supplementary Information (ESI)

Insights into the halogen-induced p-band center regulation promising high-performance lithium-sulfur batteries

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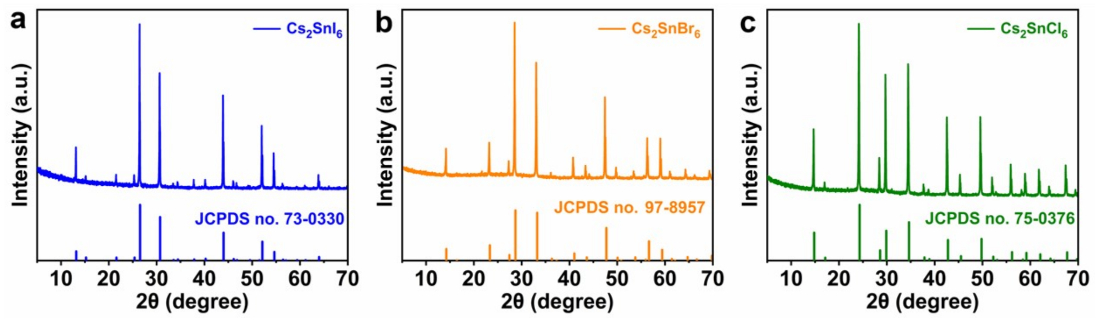

Fig. S1. XRD patterns of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6.

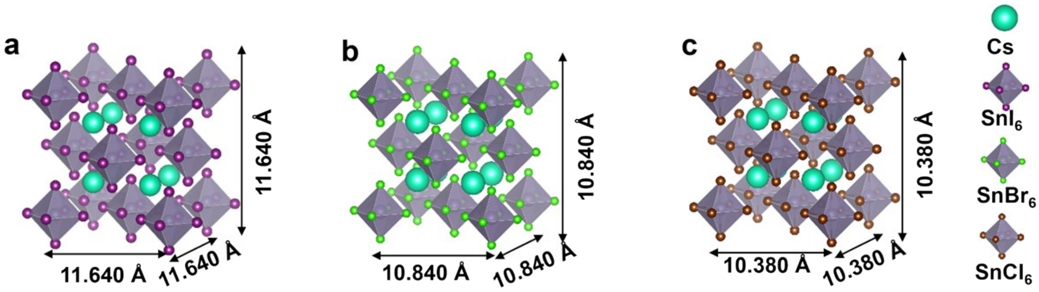

Fig. S2. Lattice parameters of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6.

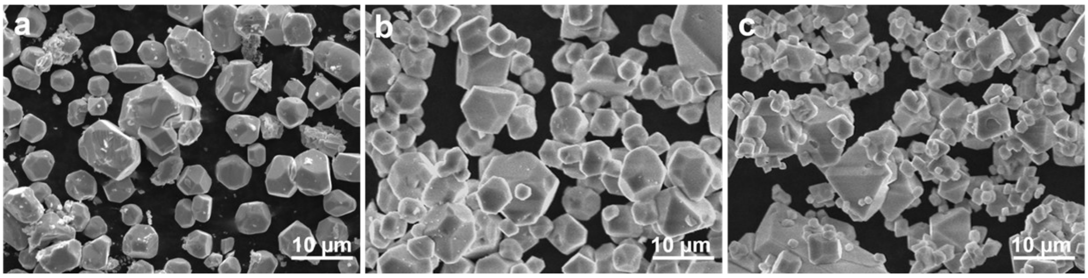

Fig. S3. FESEM images of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 before ball-milling.

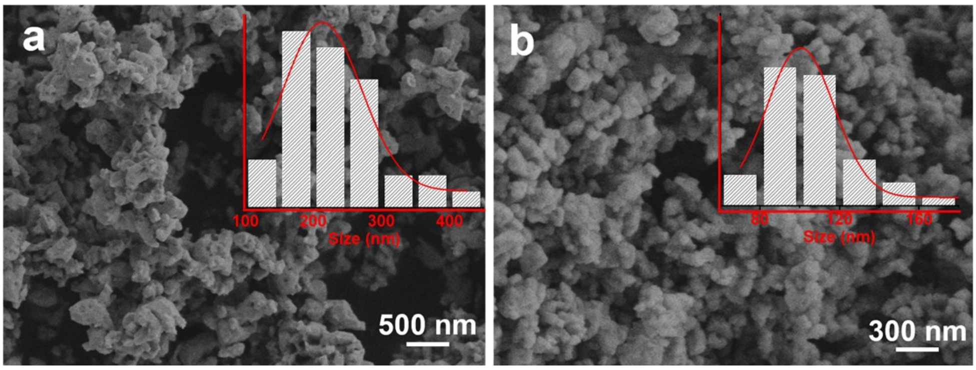

Fig. S4. FESEM images of (a) Cs_2SnBr_6 and (b) Cs_2SnCl_6 after ball-milling, and corresponding particle size distribution diagrams (the insets).

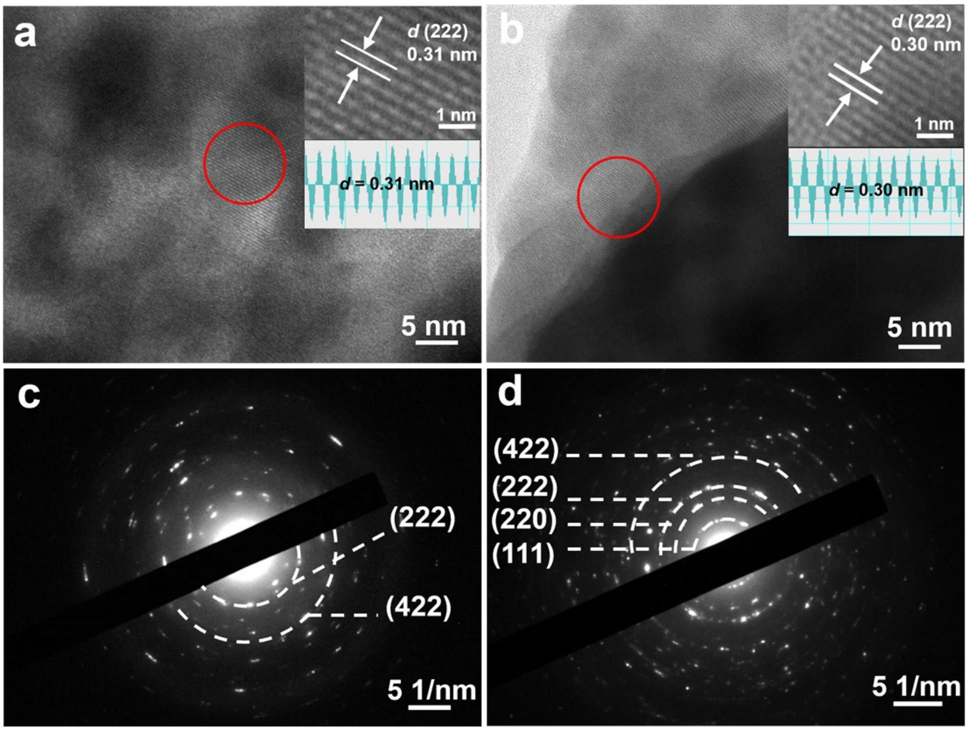

Fig. S5. (a, b) HRTEM images and (c, d) SAED patterns of Cs_2SnBr_6 and Cs_2SnCl_6.

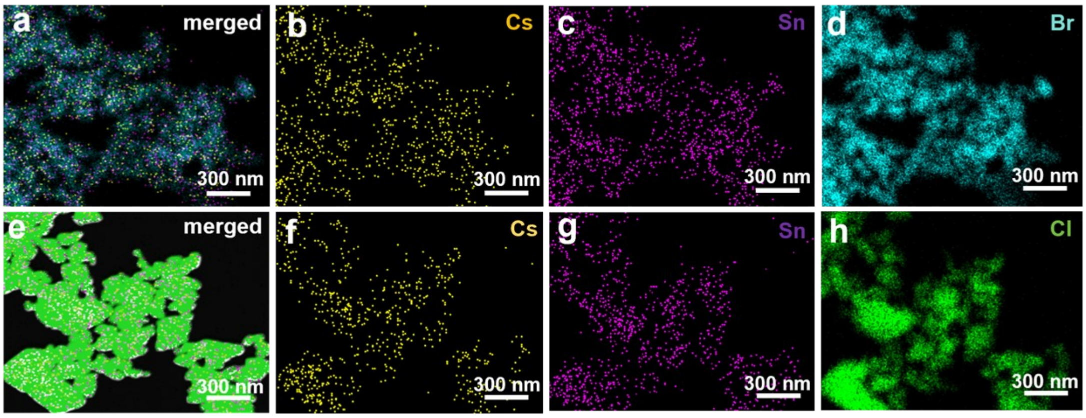

Fig. S6. EDS mapping images of Cs, Sn, and halogen elements for (a – d) Cs_2SnBr_6, and (e – h) Cs_2SnCl_6.

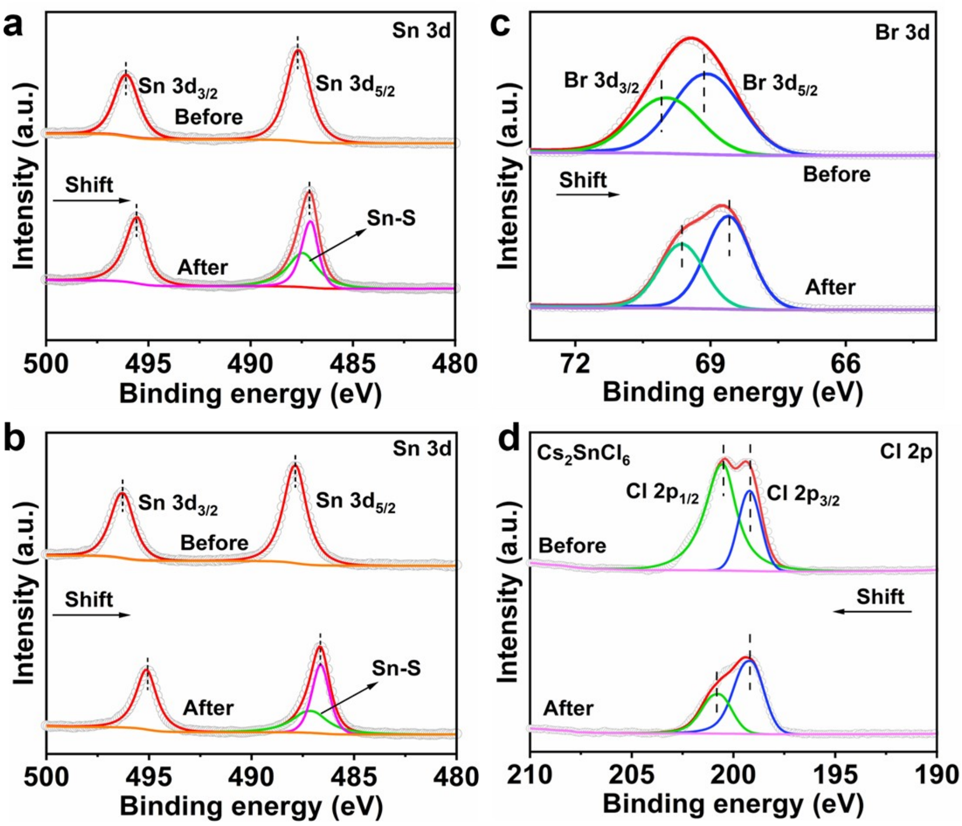

Fig. S7. Typical Sn 3d spectra of (a) Cs_2SnBr_6 and (b) Cs_2SnCl_6. (c) Br 3d spectra of Cs_2SnBr_6 and (d) Cl 2p spectra of Cs_2SnCl_6.

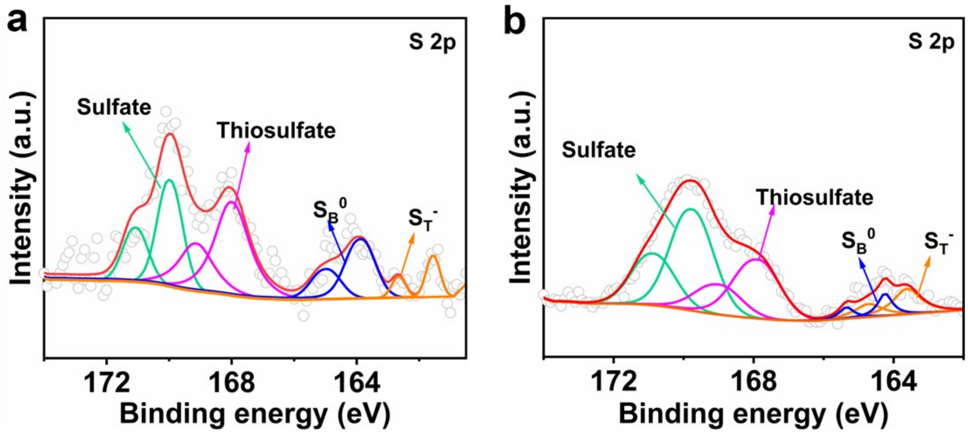

Fig. S8. S 2p spectra of (a) Cs_2SnBr_6 and (b) Cs_2SnCl_6 absorbed with Li_2S_6.

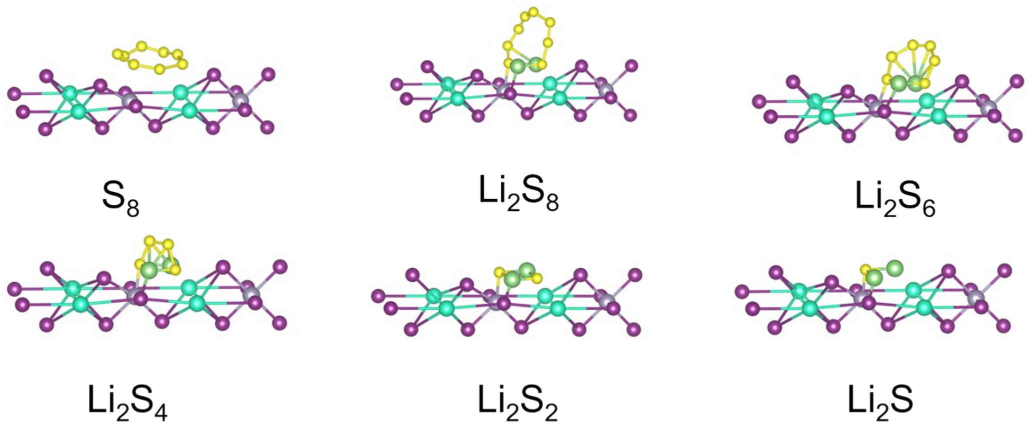

Fig. S9. Adsorption configurations of Li_2S_n ($1 \leq n \leq 8$) on the surface of Cs_2SnX_6.

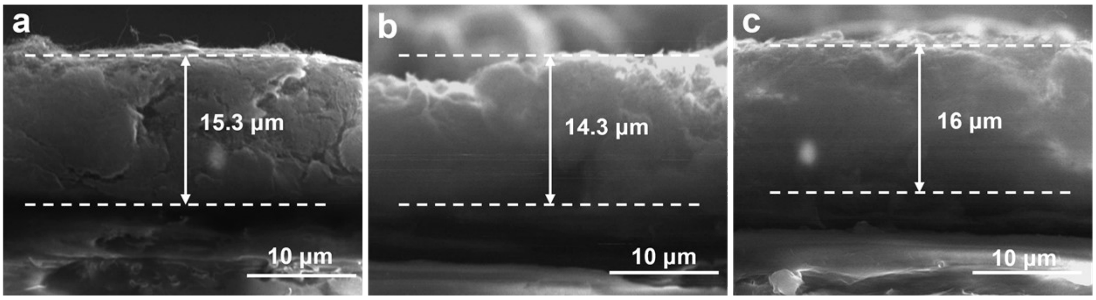

Fig. S10. Cross-sectional FESEM images of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 modified separators.

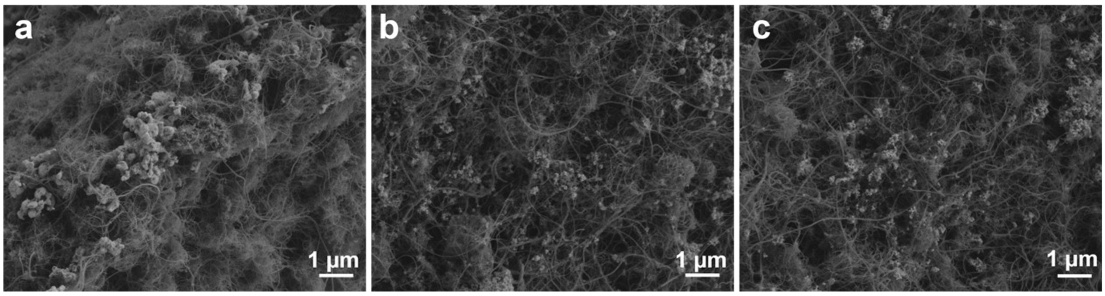

Fig. S11. Top-view FESEM images of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 modified separators.

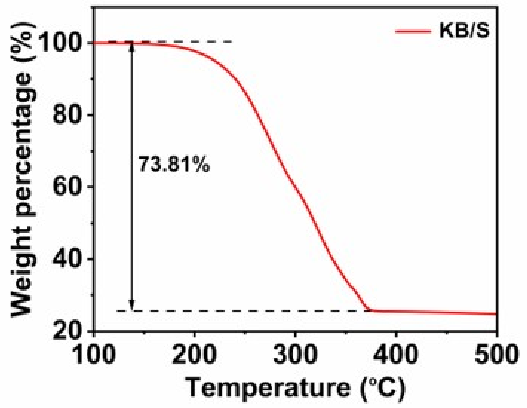

Fig. S12. Thermogravimetric analysis plot of KB/S.

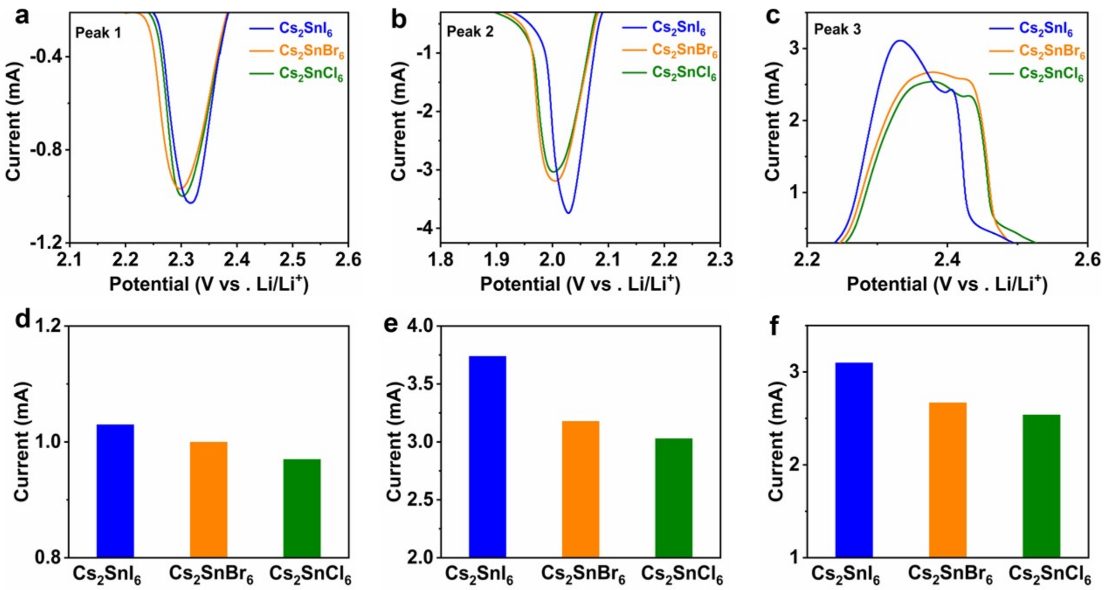

Fig. S13. (a − c) Enlarged CV curves (0.1 mV s^{-1}) and (d − f) corresponding peak current value of LSBs with Cs_2SnX_6 modified separators.

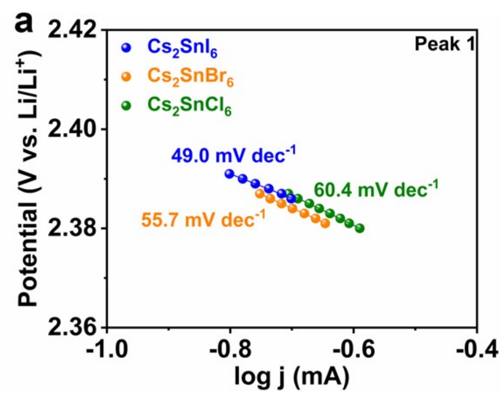

Fig. S14. Tafel slopes of (a) peak 1 and (b) peak 2 of LSBs with Cs_2SnX_6 modified separators.

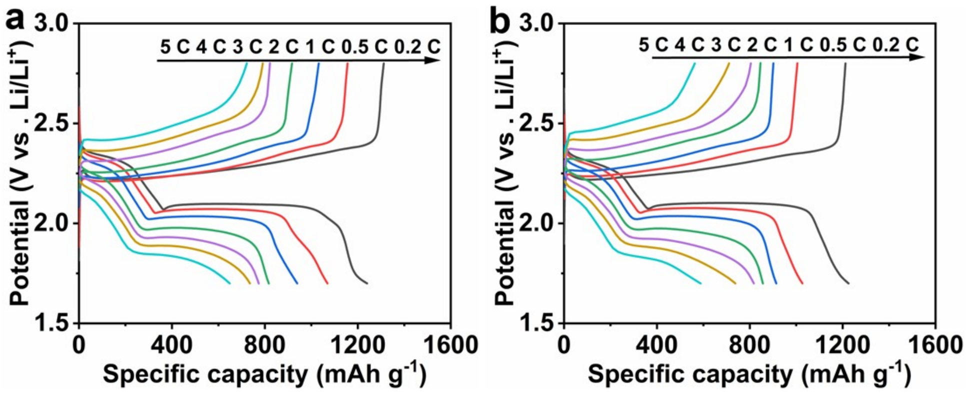

Fig. S15. Charge-discharge curves of (a) Cs_2SnBr_6 and (b) Cs_2SnCl_6 batteries at different current rates.

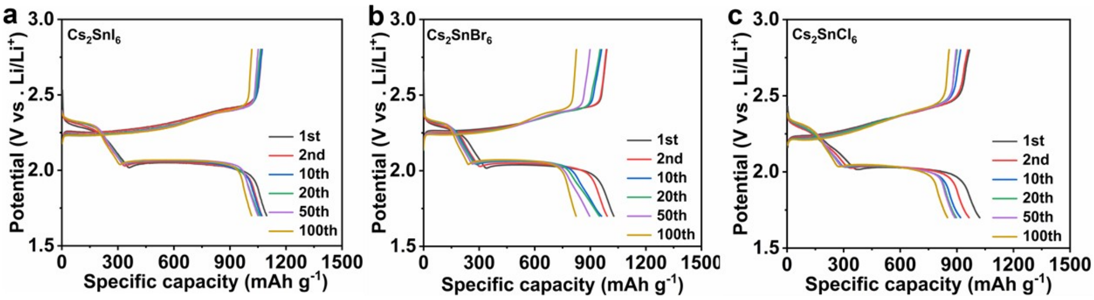

Fig. S16. Charge-discharge curves of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 batteries at different cycle times.

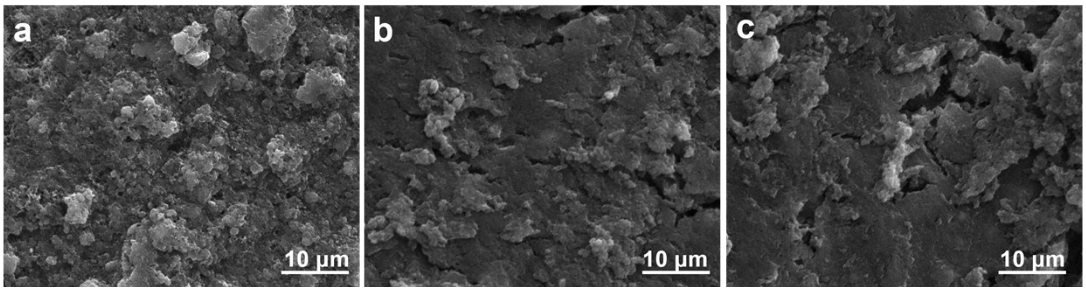

Fig. S17. FESEM images of the cathode of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 batteries after 500 cycles at 1 C.

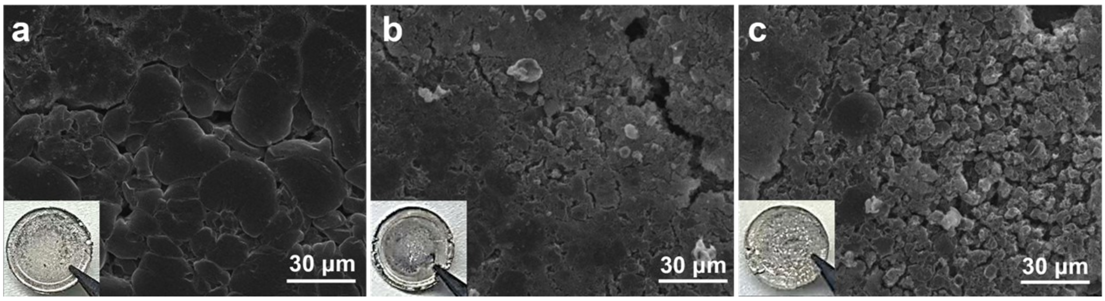

Fig. S18. FESEM images and digital photos (the insets) of lithium anodes of (a) Cs_2SnI_6, (b) Cs_2SnBr_6, and (c) Cs_2SnCl_6 batteries after 500 cycles at 1 C.

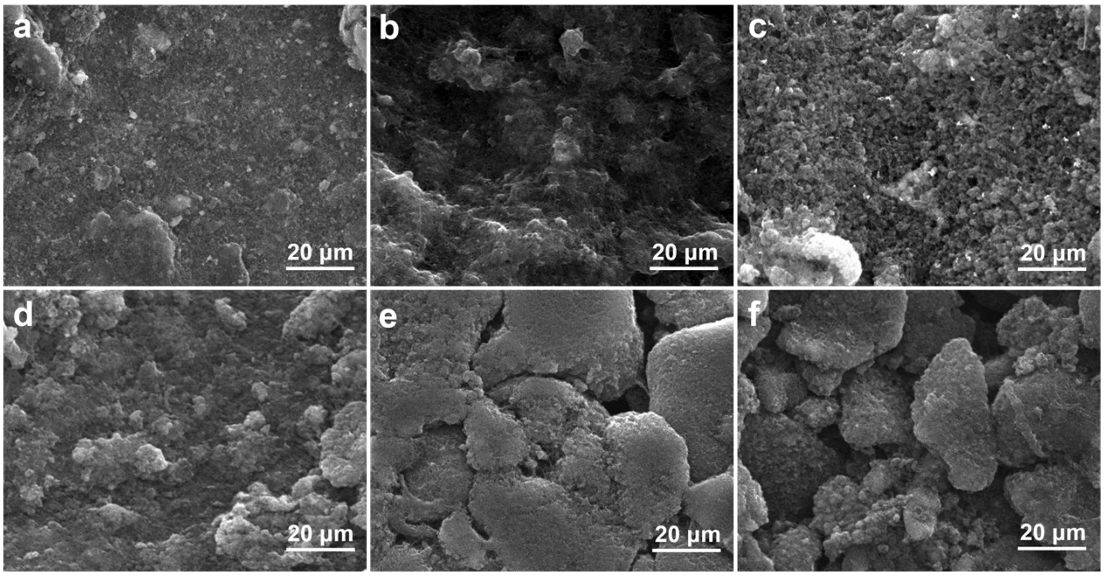

Fig. S19. FESEM images of Cs_2SnX_6 modified separators (a − c) before and (d − f) after 500 cycles at 1C.

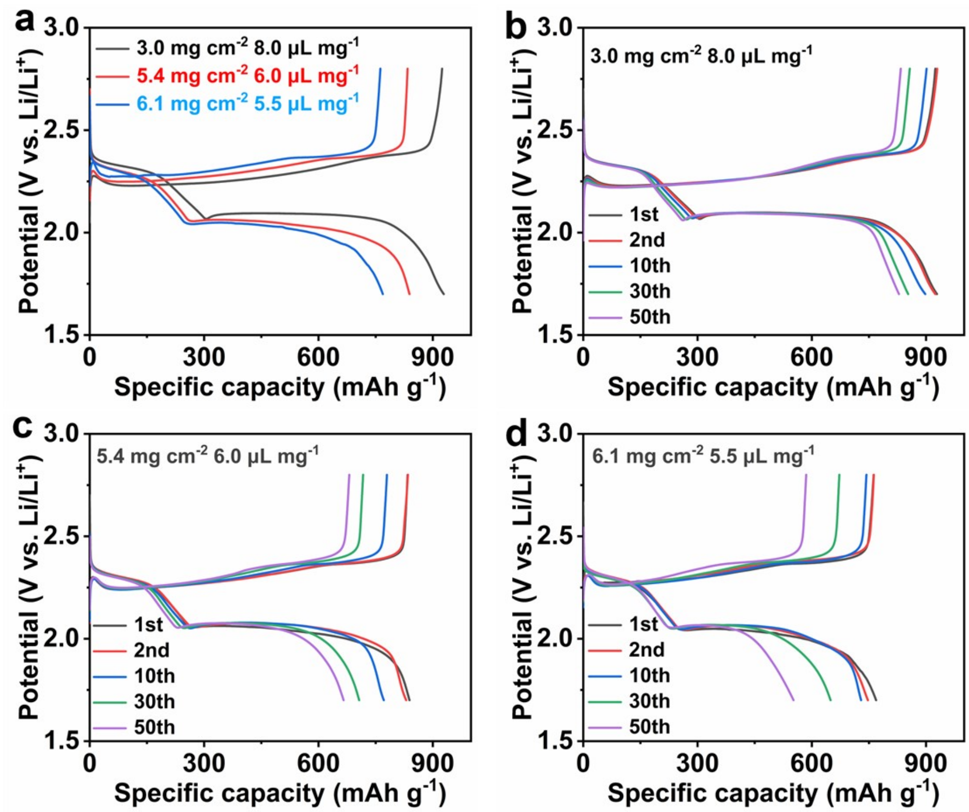

Fig. S20. (a) The first charge-discharge curves of Cs_2SnI_6 batteries under high-load and low E/S ratio conditions. (b − d) Corresponding charge-discharge curves at different cycle times as indicated.

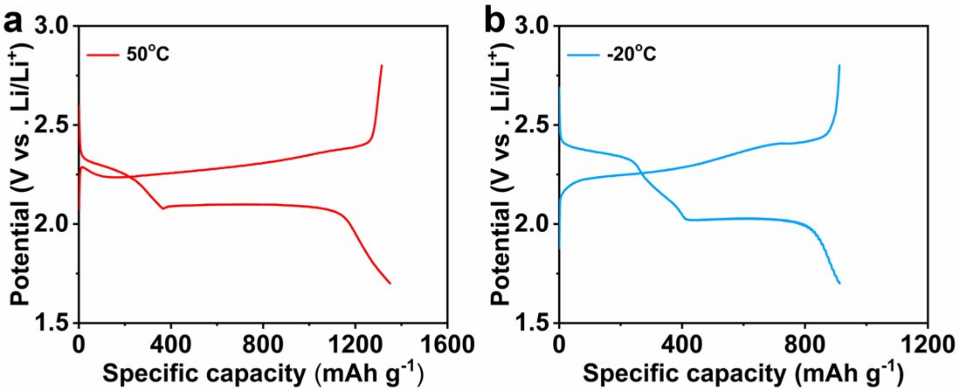

Fig. S21. The first Charge-discharge curves of Cs_2SnI_6 batteries in environments of 50℃ (0.5 C) and –20 ℃ (0.1 C).

Table S1 EIS fitting results of Cs_2SnX_6 batteries.

	Coated materials	R_s (Ω)	R_{sf} (Ω)	R_{ct} (Ω)
Before cycling	Cs_2SnCl_6	1.6	-	73.5
	Cs_2SnBr_6	1.8	-	72.6
	Cs_2SnI_6	2.9	-	60.7
After cycling	Cs_2SnCl_6	3.9	20.6	7.6
	Cs_2SnBr_6	3.5	17.7	6.2
	Cs_2SnI_6	4.5	13.8	2.9

Table S2. Performance comparison of LSBs with various separators.

Coated materials	Current rate (C)	Cycle number	Capacity decay per cycle (%)
Cs_2SnI_6 (This work)	**2**	**500**	**0.068**
VN@NG [1]	2	500	0.075
CQDs-PAN [2]	0.5	500	0.075
H-CMP [3]	1	500	0.066
Li-MOF/RGO [4]	1	600	0.089
Zwitterionic COF [5]	2	500	0.072
C_3N_4-$CoSe_2$ [6]	1	500	0.089
ZIF-8 [7]	1	500	0.100
Ni/SiO2/G [8]	1	300	0.086
Co/Mo_2C [9]	1	600	0.072

Table S3 Performance comparison of LSBs with various separators under high-load and low-E/S-ratio conditions.

Coated materials	Sulfur loading ($mg\ cm^{-2}$)	E/S ratio ($\mu l\ mg^{-1}$)	Initial specific capacity ($mAh\ g^{-1}$) @ C rates
Cs_2SnI_6 (This work)	**6.10**	**5.5**	**768.8@0.2 C**
NbB_2/rGo [10]	7.06	10	590.7@0.1 C
Co-MoS_2 [11]	5.27	12	800.8@0.2 C
NS-MXene [12]	7.20	7.0	730.6@0.2 C
Fe-ZIF-8 [13]	5.00	5.0	517@0.05 C
TpPa-SO_3H [14]	5.00	10	800.0@0.2 C
ZIF-67/SA-PAN [15]	5.45	10	797.5@0.1 C
ZrO_2-SiO_2 [16]	4.00	10	757.0@0.2 C
GQDs-PAN [17]	5.10	15	633.3@0.1 C
RPM [18]	5.40	10	703.7@0.2 C

Table S4. Performance comparison of LSBs with various separators under different operating temperatures

Coated materials	Temperature (°C)@Current rate (C)@Initial specific capacity (mAh g^{-1})
Cs_2SnI_6 (This work)	**-20 °C@0.1 C@ 912.7 mAh g^{-1}** **50 °C@0.5 C@1350 mAh g^{-1}**
Go-CoNiP [19]	-20 °C@0.5 C@810.9 mAh g^{-1} 60 °C@0.5 C@1064.8 mAh g^{-1}
SAF-3 [20]	-20 °C@0.1 C@870.0 mAh g^{-1} 60 °C@0.5 C@1064.8 mAh g^{-1}
NbB_2 [21]	-10 °C@0.1 C@802.0 mAh g^{-1}
TPE [22]	-20 °C@0.1 C@802.0 mAh g^{-1}
FeCoNi [23]	0 °C@0.2 C@931.0 mAh g^{-1}
Fe/Ni-N@NC [24]	0 °C@0.5 C@741.0 mAh g^{-1}

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