

Supporting Information

Progress and Perspectives of Halide-based Lithium Conductors for All-Solid-State Batteries

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Table S1. Parameters of the selected electrode systems.

Electrode materials system	Average Voltage (V)	Cathode			Anode		
		Press Density (g cm ⁻³)	Reversible Capacity (mAh g ⁻¹)	Initial Coulombic Efficiency	Press Density (g cm ⁻³)	Reversible Capacity (mAh g ⁻¹)	Initial Coulombic Efficiency
LCO/Li	3.95	4.2 (96.5wt%)	190	97%	0.53	3860	100%
		4.031 (90wt%)					
		3.901 (90wt%)					
Li rich/Li	4	2.7 (96.5wt%)	300	90%	0.53	3860	100%
		2.6285 (90wt%)					
		2.5735 (90wt%)					
NMC811/Li	3.8	3.5 (96.5wt%)	210	90%	0.53	3860	100%
		3.3765 (90wt%)					
		3.2815 (90wt%)					
S/Li	2	0.8609 (70wt%)	1336	100%	0.53	3860	100%
		0.7077 (60wt%)					
		0.6007 (50wt%)					

The reversible capacity of S cathode is 80% of its theoretical capacity. 15% porosity is considered to moderate volume change. The mass ratio of S: PVDF: Super P = x% : 2(1-x%)/3 : (1-x%)/3. The density of PVDF and Super P is 0.8 g cm⁻³ and 0.16 g cm⁻³, respectively.

Table S2. Parameters of the selected SSE systems.

Electrolyte	Density (g cm ⁻³)
LGPS	2.05
Li ₃ InCl ₆	2.59
LLZO	5.07
PEO	1.24
Li ₃ ErCl ₆	3.07
Li ₃ ScCl ₆	2.18

Table S3. Typical technological parameters of an NMC811/Li pouch cell with a fixed size of 138 mm × 81.8 mm × 7.13 mm.

Component of Cell	Parameter	Value
Cathode	Material	NMC811
	Reversible capacity (mAh g ⁻¹)	210
	Initial Coulombic efficiency (%)	90
	Unilateral areal density (mg cm ⁻² each side of Al)	22.925
	Active material ratio (%)	96.5
	Press density (g cm ⁻³)	3.5
	Unilateral thickness (μm)	65.5
	Thickness of Al (μm)	16
	Length (mm)	120
	Width (mm)	73
	layer	22
Anode	Material	Li
	Reversible capacity (mAh g ⁻¹)	3860
	Initial Coulombic efficiency (%)	100
	Unilateral areal density (mg cm ⁻² each side of Cu)	2.407125
	Active material ratio (%)	100
	Press density (g cm ⁻³)	0.53
	Unilateral thickness (μm)	45.41745
	Thickness of Cu (μm)	8
	Length (mm)	123
	Width (mm)	76
	layer	23

Electrolyte	Material	Li_3InCl_6
	Thickness (μm)	30
	Length (μm)	126
	Width (μm)	76
	layer	44
Sealing film	Thickness (μm)	152
Cell	Voltage (V)	3.8
	Capacity (Ah)	17.90658
	Mass (g)	165.879
	Volume (L)	0.0805
	Gravimetric energy density (Wh kg^{-1})	410.2084
	Volumetric energy density (Wh L^{-1})	845.2811

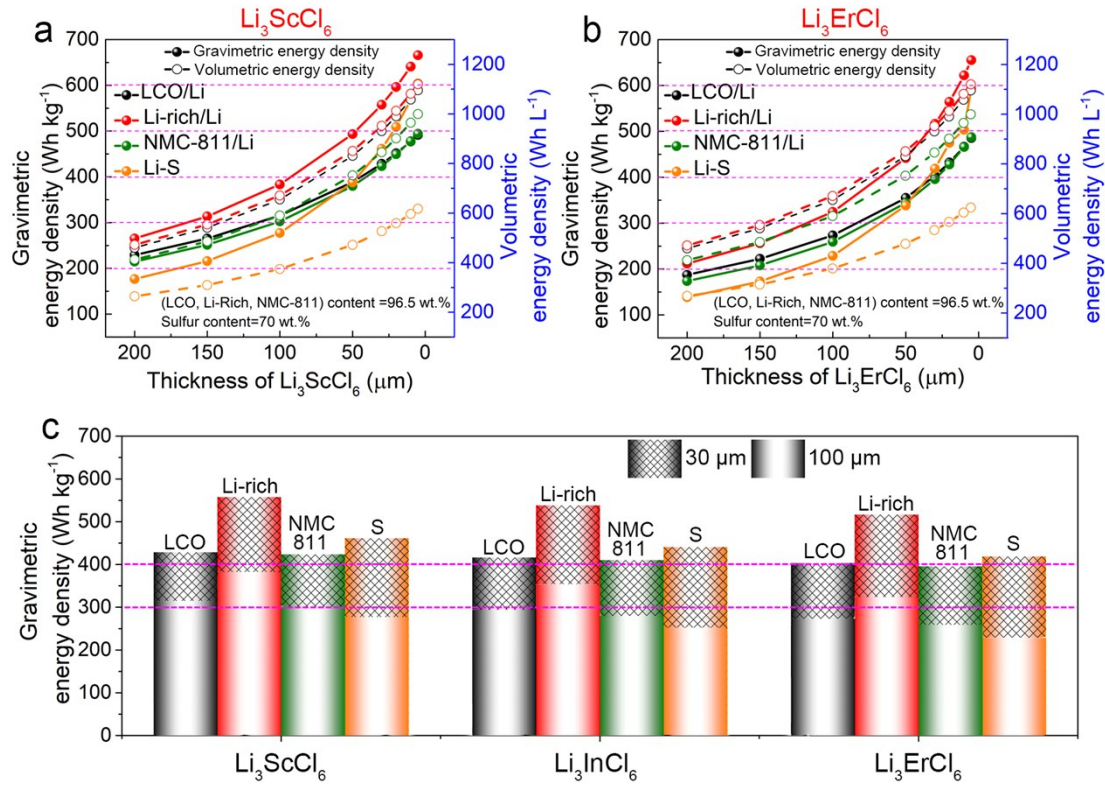


Figure S1. Gravimetric/volumetric energy densities of ASSLBs as a function of halide SSE thickness. (a) Li_3ScCl_6 and (b) Li_3ErCl_6 . (c) The gravimetric energy densities of ASSLBs based on two representative thicknesses (30 μm and 100 μm) of SSE; the black, red, green, and yellow colors refer to LCO, Li-rich, NMC811, and S cathodes, respectively. The weight percentage of

the active materials is 96.5 wt% for LCO, Li-rich, and NMC-811 cathodes and 70 wt% for S cathode. The calculation details are provided in the Supplemental Information.

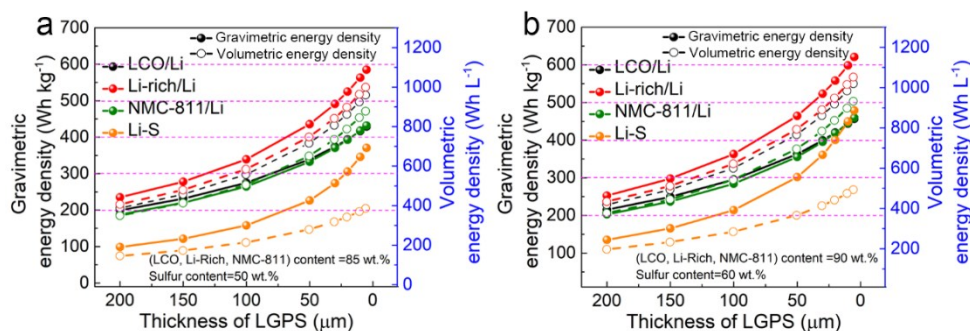


Figure S2. Gravimetric/volumetric energy densities of ASSLBs as a function of LGPS SSE thickness. (a) The weight percentage of the active materials is 85 wt% for LCO, Li-rich, and NMC811 cathodes and 50 wt% for S cathode, (b) the weight percentage of the active materials is 90 wt% for LCO, Li-rich, and NMC811 cathodes and 60 wt% for S cathode.

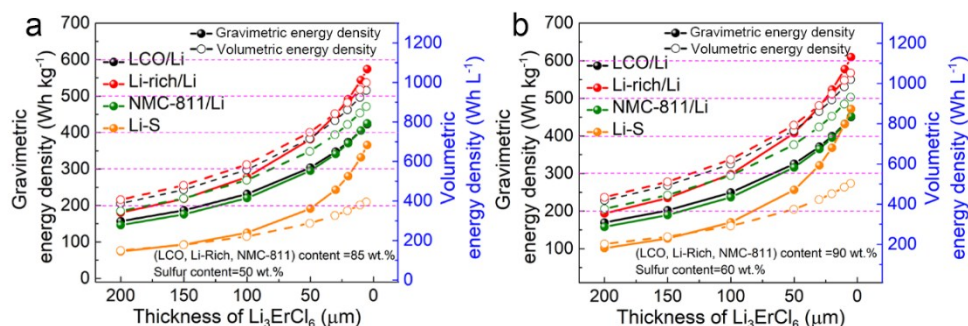


Figure S3. Gravimetric/volumetric energy densities of ASSLBs as a function of Li_3ErCl_6 SSE thickness. (a) The weight percentage of the active materials is 85 wt% for LCO, Li-rich, and NMC811 cathodes and 50 wt% for S cathode, (b) the weight percentage of the active materials is 90 wt% for LCO, Li-rich, and NMC811 cathodes and 60 wt% for S cathode.

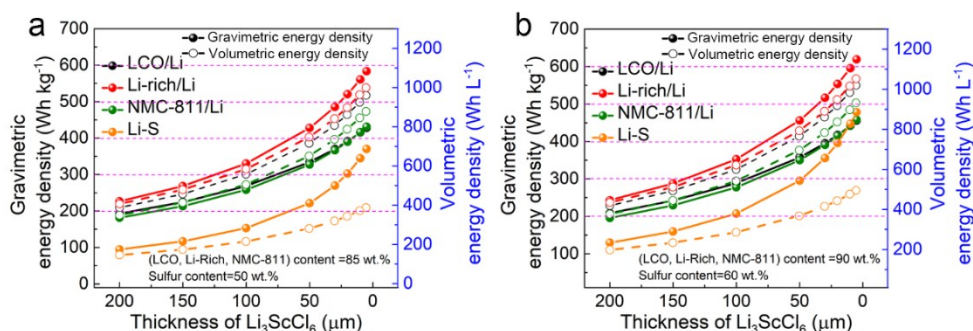


Figure S4. Gravimetric/volumetric energy densities of ASSLBs as a function of Li_3ScCl_6 SSE thickness. (a) The weight percentage of the active materials is 85 wt% for LCO, Li-rich, and NMC811 cathodes and 50 wt% for S cathode, (b) the weight percentage of the active materials is 90 wt% for LCO, Li-rich, and NMC811 cathodes and 60 wt% for S cathode.

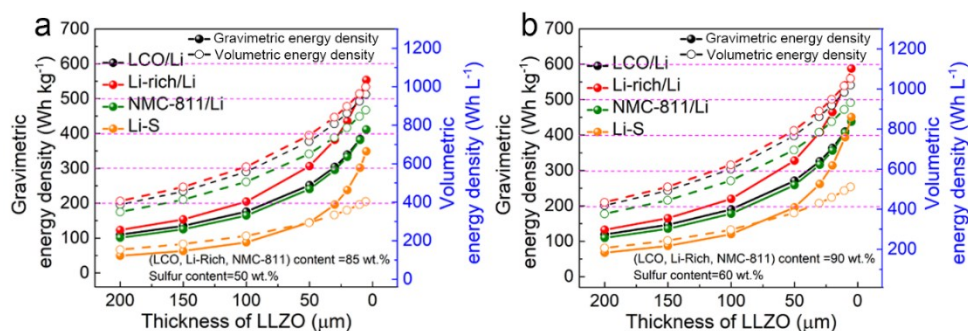


Figure S5. Gravimetric/volumetric energy densities of ASSLBs as a function of LLZO SSE thickness. (a) The weight percentage of the active materials is 85 wt% for LCO, Li-rich, and NMC811 cathodes and 50 wt% for S cathode, (b) the weight percentage of the active materials is 90 wt% for LCO, Li-rich, and NMC811 cathodes and 60 wt% for S cathode.

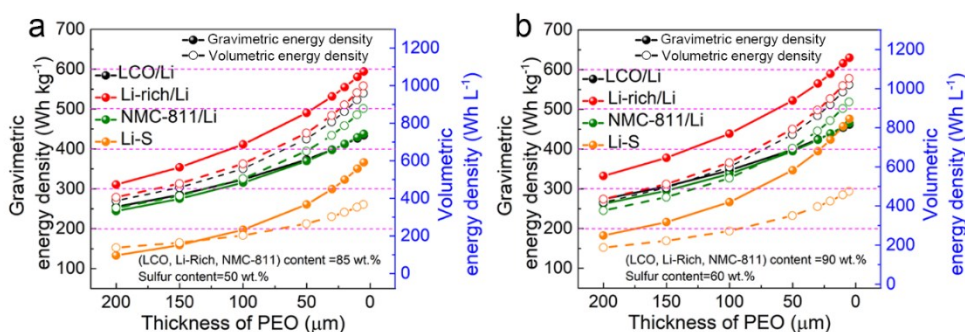


Figure S6. Gravimetric/volumetric energy densities of ASSLBs as a function of PEO SSE thickness. (a) The weight percentage of the active materials is 85 wt% for LCO, Li-rich, and

NMC811 cathodes and 50 wt% for S cathode, (b) the weight percentage of the active materials is 90 wt% for LCO, Li-rich, and NMC811 cathodes and 60 wt% for S cathode.