



Supplementary Information

Cl- and Al-Doped Argyrodite Solid Electrolyte $\text{Li}_6\text{PS}_5\text{Cl}$ for All-Solid-State Lithium Batteries with Improved Ionic Conductivity

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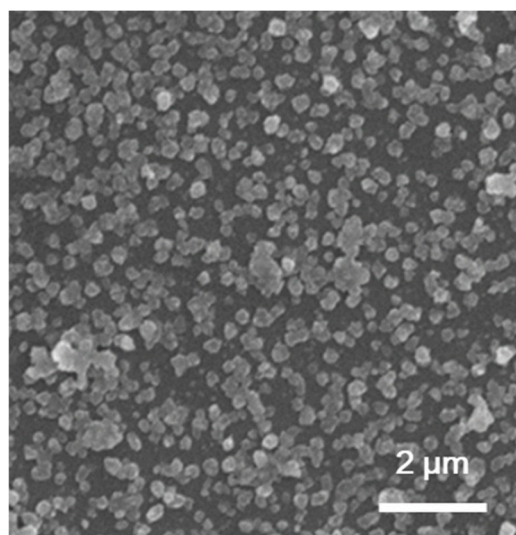


Figure S1. FE-SEM images of $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolytes.

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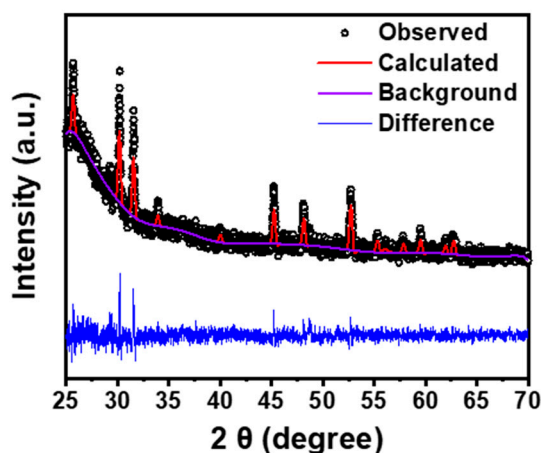


Figure S2. XRD pattern of and the corresponding Rietveld refinement of $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolyte.

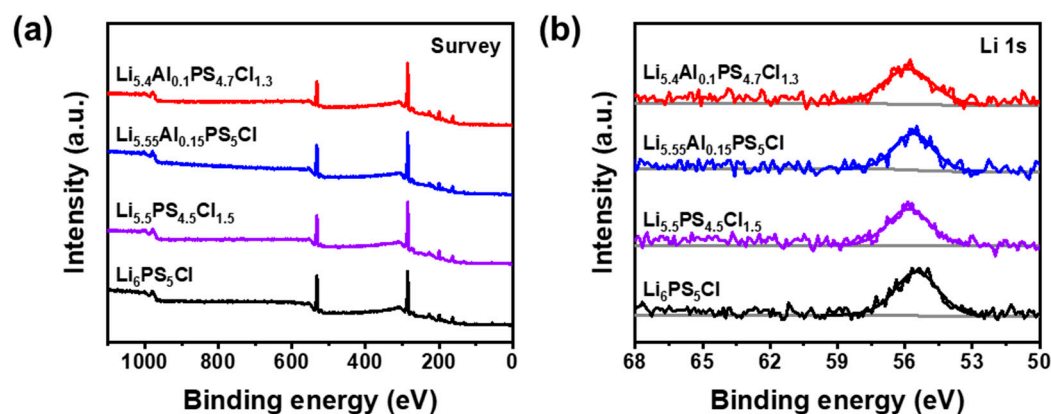


Figure S3. XPS spectra of $\text{Li}_6\text{PS}_5\text{Cl}$, $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$, $\text{Li}_{5.55}\text{Al}_{0.15}\text{PS}_5\text{Cl}$, and $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolytes for (a) Survey, and (b) Li 1s.

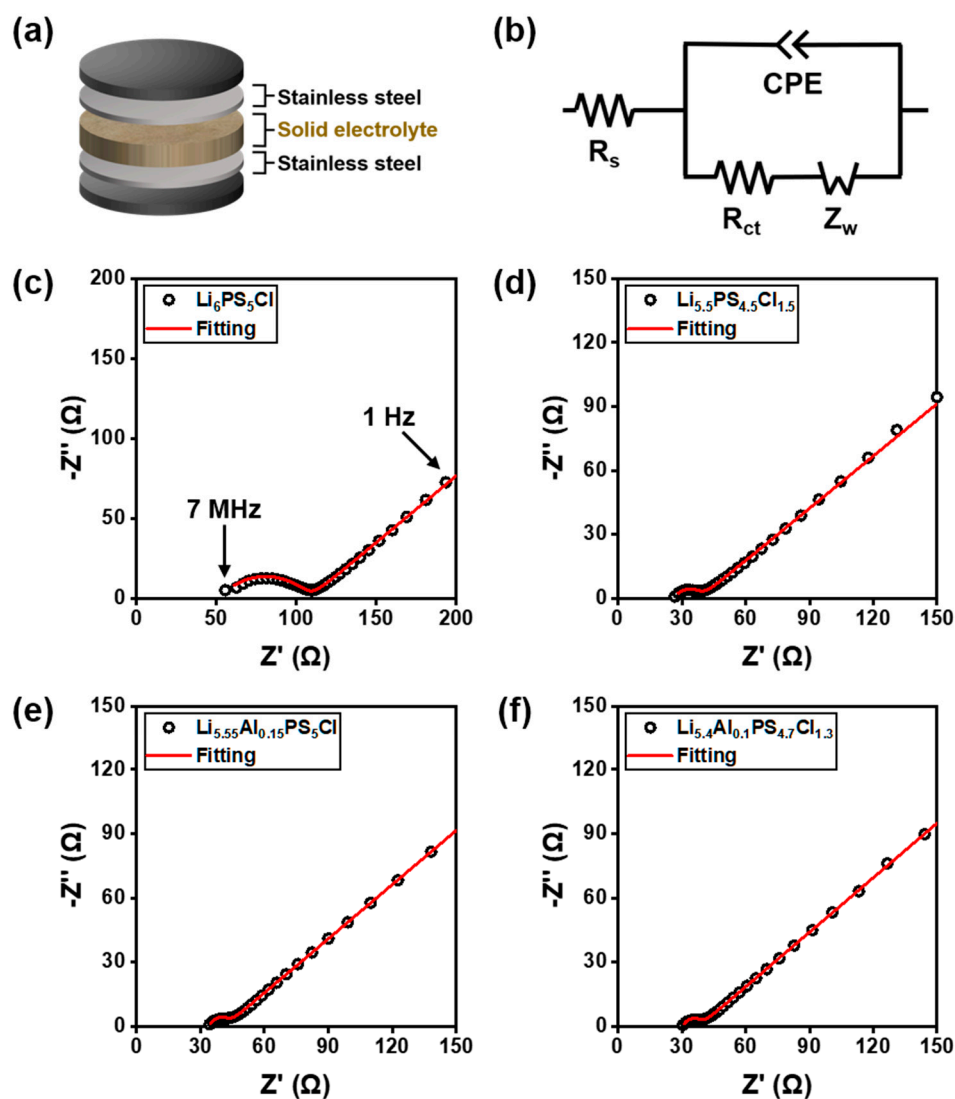


Figure S4. (a) Schematic diagram of cell geometry for impedance measurement. (b) Equivalent circuit for modeling the EIS data. Nyquist plots of (c) $\text{Li}_6\text{PS}_5\text{Cl}$, (d) $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$, (e) $\text{Li}_{5.55}\text{Al}_{0.15}\text{PS}_5\text{Cl}$, and (f) $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolytes, respectively. Experimental data (circles) was fitted with the simulated data from equivalent circuit modeling (lines).

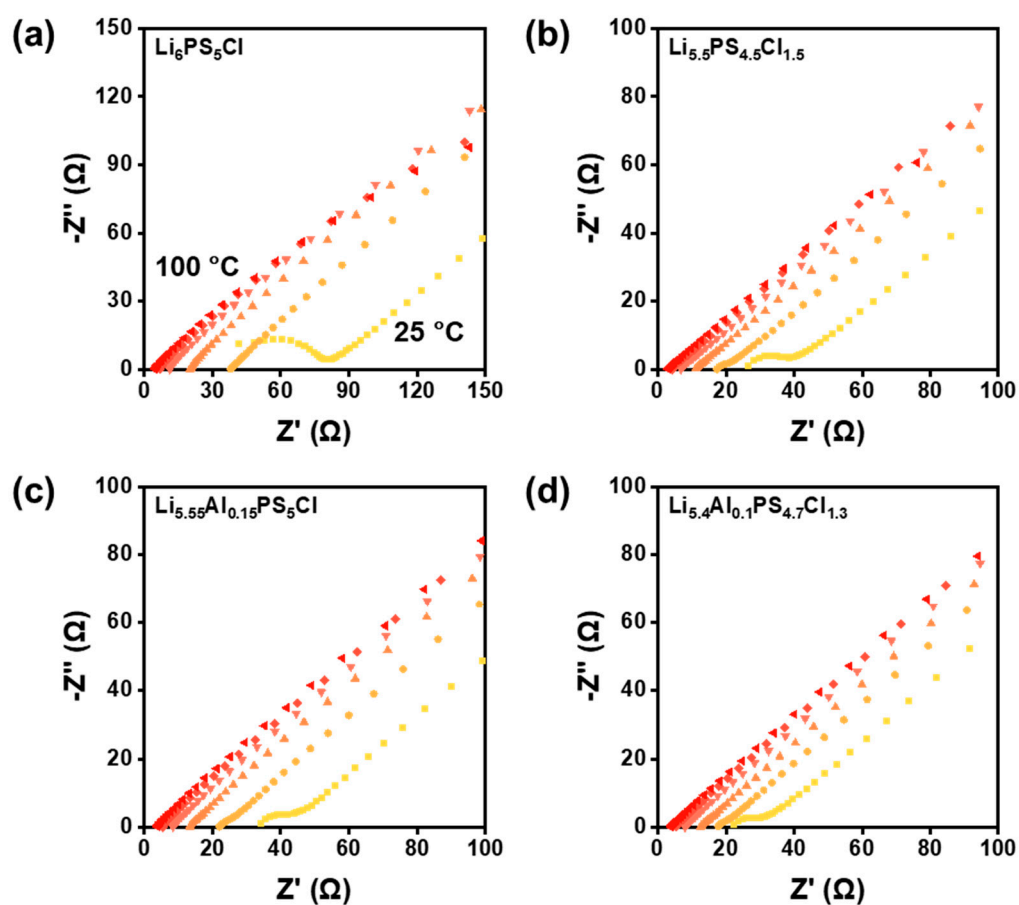


Figure S5. Nyquist plots of the (a) $\text{Li}_6\text{PS}_5\text{Cl}$, (b) $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$, (c) $\text{Li}_{5.55}\text{Al}_{0.15}\text{PS}_5\text{Cl}$, and (d) $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolytes measured from 25 to 100 °C, respectively.

Table S1. Rietveld refinements data of $\text{Li}_{5.4}\text{Al}_{0.1}\text{PS}_{4.7}\text{Cl}_{1.3}$ electrolyte.

space group $F\bar{4}3m$, $a=10.28 \text{ \AA}$, $R_{wp}=19.51 \%$						
atom	site	x	y	z	OCC.	Uiso (\AA^2)
Li1	24g	0.25	0.25	0.36369	1	-2.62899
P1	4b	0.5	0	0	1	0.05134
S1	4a	0.25	0.25	0.25	1	-1.02402
S2	4c	0.12684	0.37316	0.87316	1	-0.05982
Cl1	4a	0	0	0	1	-0.11452