Supporting Information for: $Li_{15}P_4S_{16}Cl_3$, a lithium chloro-thiophosphate as a solid-state ionic conductor

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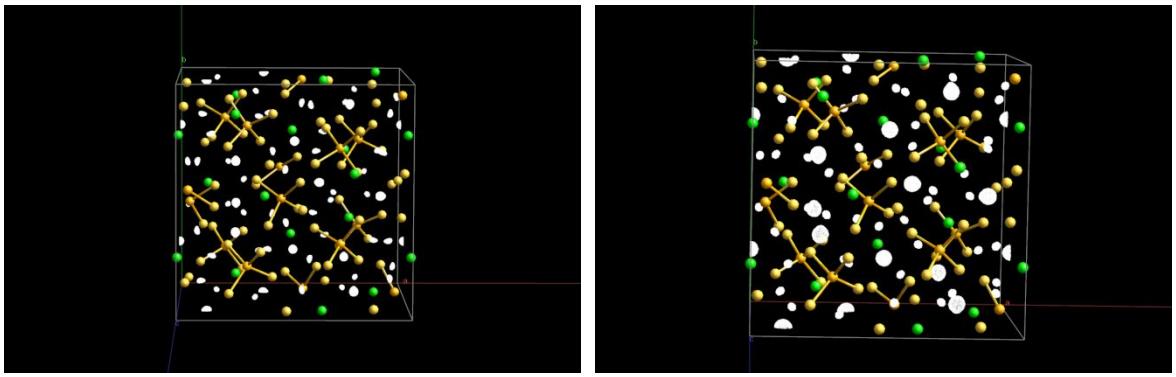

Figure S1. Difference Fourier maps used to identify Li sites generated from synchrotron X-ray diffraction data (left, where white regions indicate positive difference peaks associated with the Li electron density) and time-of-flight neutron diffraction data (right, where white regions indicate negative peaks associated with the Li coherent nuclear scattering length density). The residual positions from both X-ray diffraction and neutron diffraction matches well with the refined positions from Rietveld refinement.

Table S1. Refined structure of $Li_{15}P_4S_{16}Cl_3$ using synchrotron diffraction data (λ = 0.24116 Å).

S.G. *I*-43d a = 14.3066(4) Å

Site	Wyck.	x	y	z	Occ.	B_{iso} (Å^2)
Li(1)	12a	0.00000	0.25000	0.37500	1	3.65(48)
Li(2)	48e	0.1427(13)	0.2082(15)	0.5921(19)	1	3.65(48)
S(1)	16c	0.0322(2)	0.0322(2)	0.0322(2)	1	1.35(7)
S(2)	48e	0.1086(2)	0.3428(3)	0.4721(2)	1	1.35(7)
Cl(1)	12b	0.00000	0.25000	0.87500	1	2.23(17)
P(1)	16c	0.1996(2)	0.1996(2)	0.1996(2)	1	1.18(13)

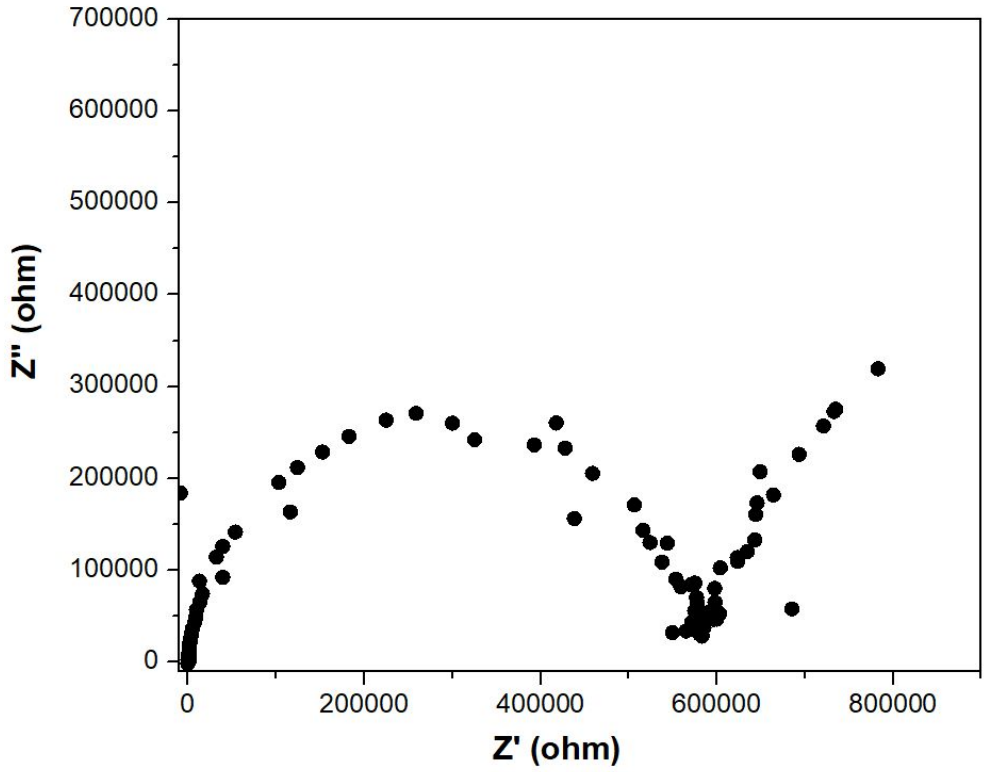

Fig. S2. Nyquist plot of $Li_{15}P_4S_{16}Cl_3$ at 30 °C.

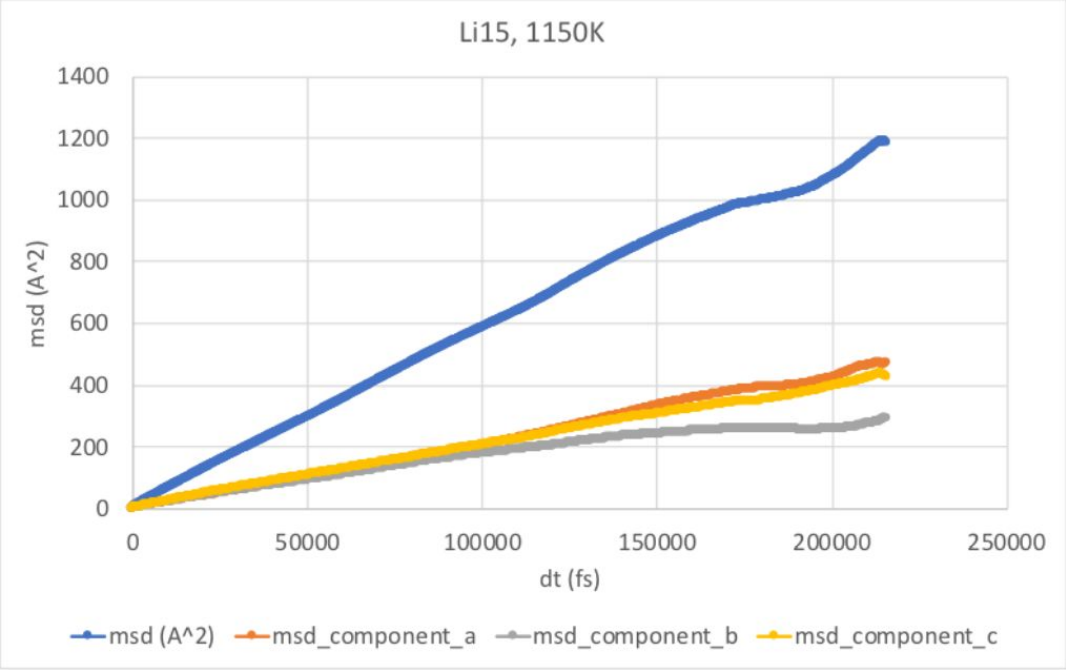

Fig. S3. The Mean-squared Displacement-time (MSD-t) relationship