

Supplementary information

A Facile Strategy to Achieve High Conduction and Excellent Chemical Stability of Lithium

Solid Electrolytes

Shufeng Song, Jia Lu, Feng Zheng, Hai M. Duong*, and Li Lu*

Materials Science Group, Department of Mechanical Engineering National University of

Singapore, Singapore 117575

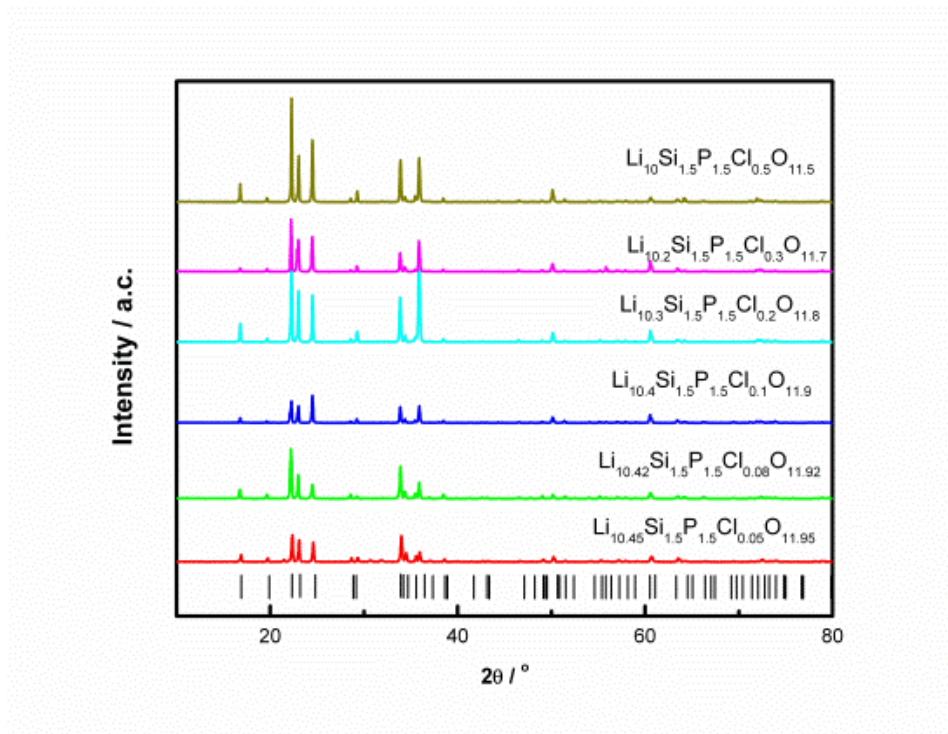


Figure S1. XRD patterns of $\text{Li}_{10.5-x}\text{Si}_{1.5}\text{P}_{1.5}\text{Cl}_x\text{O}_{12-x}$ ($0.05 \leq x \leq 0.5$). The short vertical lines below the profiles mark the peaks positions of $\gamma\text{-Li}_3\text{PO}_4$ (PDF 15-0760).

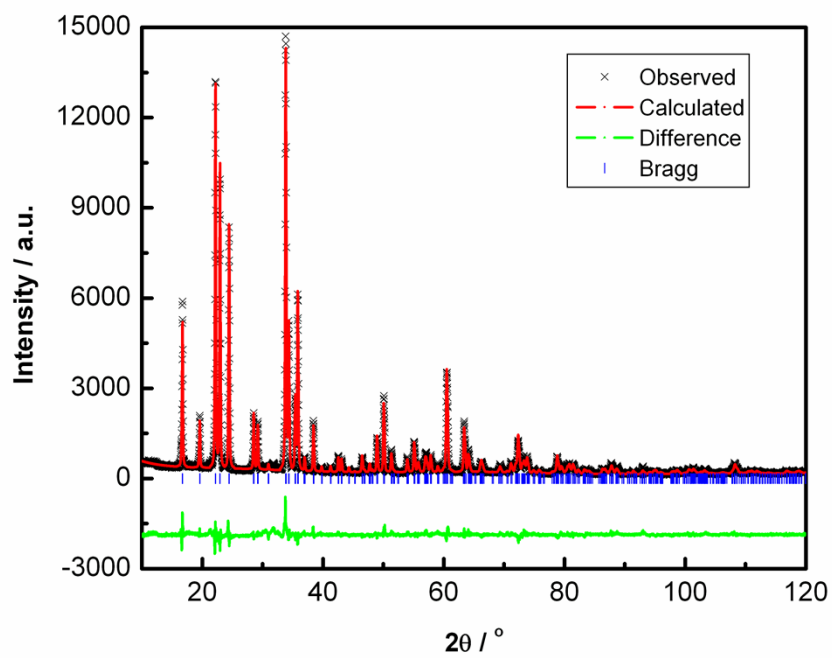


Figure S2. Typical observed, calculated, and difference patterns for Rietveld refinement of $\text{Li}_{10}\text{Si}_{1.5}\text{P}_{1.5}\text{Cl}_{0.5}\text{O}_{11.5}$.

Table S1 Crystallographic data of $\text{Li}_{10}\text{Si}_{1.5}\text{P}_{1.5}\text{Cl}_{0.5}\text{O}_{11.5}$ from Rietveld refinement of powder**XRD data**

Atom	Site	x, y, z	Occupancy	U_{iso}
Li1	8d	0.29344(1), 0.50060(8), 0.17261(5)	1.0	0.0575(9)
Li2	4c	0.17171(3), 0.75, 0.44964(3)	1.0	0.0507(5)
Li3	8d	0.02943(3), 0.42520(1), 0.12463(8)	0.166(3)	0.0231(6)
P	4c	0.35169(4), 0.25, 0.41858(5)	0.5	0.0251(6)
Si	4c	0.31284(5), 0.25, 0.41102(7)	0.5	0.0023
O1	8d	0.22783(2), 0.03067(6), 0.33983(1)	0.916(3)	0.0062(5)
O2	4c	0.28485(3), 0.25, 0.05236(2)	1.0	0.0122(4)
O3	4c	0.15289(4), 0.75, 0.08424(5)	1.0	0.0131(6)
Cl	8d	0.00554(6), 0.01025(6), 0.35014(3)	0.083(8)	0.0969(9)
R_{wp}		0.0787		
R_{p}		0.0638		
CHI^2		4.416		