

Supporting Information for

Effect of Fluorine Substitution in Li_3YCl_6 Chloride Solid Electrolytes for All-solid-state Battery

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Figure S1: Diffraction peak broadening by fluorine substitution to Li_3YCl_6 .

Figure S2: Ionic conductivity measurements of fluorine-substituted Li_3YCl_6 .

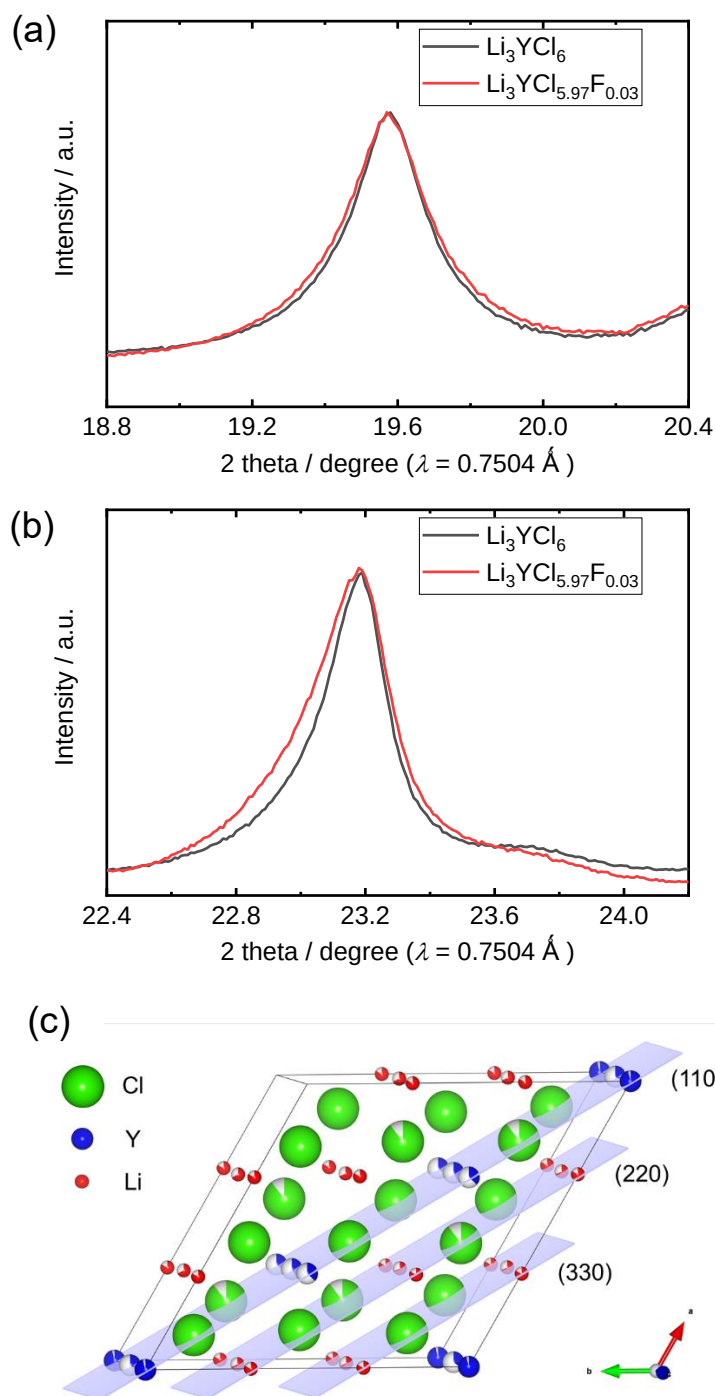


Figure S1. Enlarged synchrotron X-ray diffraction peaks of (a) 302 and (b) 330 diffraction lines. Broadening of diffraction peaks is observed, especially in the 330-diffraction line. (c) The schematic illustration of Li_3YCl_6 crystal structure with (110), (220) and (330) planes. Chloride ions are arranged on each plane. Fluoride ions with large difference in ionic radius from chloride ions induced local distortion on chloride sites.

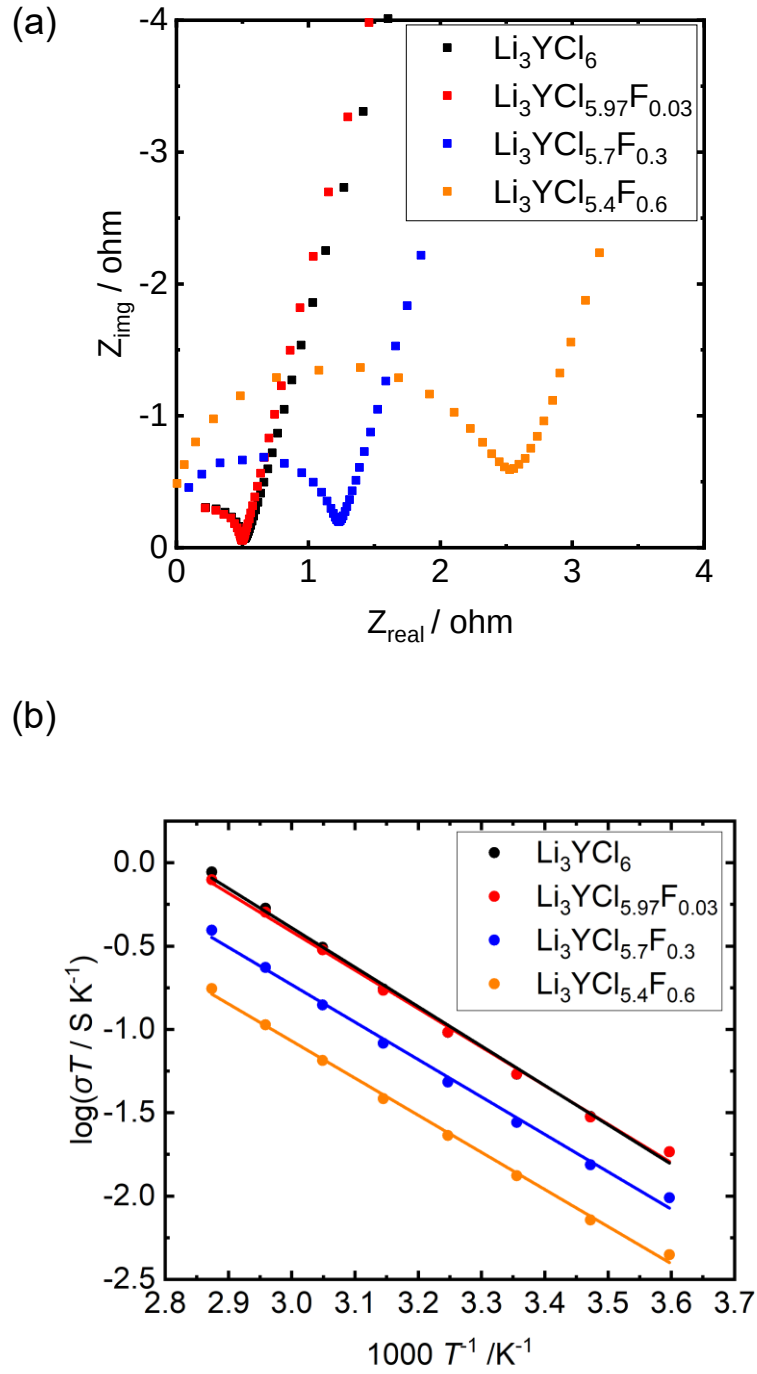


Figure S2. Comparison of ionic conductivities of various amounts of fluorine substitution to Li_3YCl_6 electrolytes. (a) Nyquist plots from the electrochemical impedance spectroscopy of Li_3YCl_6 , $\text{Li}_3\text{YCl}_{5.97}\text{F}_{0.03}$, $\text{Li}_3\text{YCl}_{5.7}\text{F}_{0.3}$ and $\text{Li}_3\text{YCl}_{5.4}\text{F}_{0.6}$ in 298 K. (b) Arrhenius plots for the ionic conductivity (σ) times temperature (T) of Li_3YCl_6 , $\text{Li}_3\text{YCl}_{5.97}\text{F}_{0.03}$, $\text{Li}_3\text{YCl}_{5.7}\text{F}_{0.3}$ and $\text{Li}_3\text{YCl}_{5.4}\text{F}_{0.6}$ in the temperature range of 278 to 348 K.