Supporting Information X-ray Pair Distribution Function Analysis, Electrical and Electrochemical Properties of Cerium Doped Li₅La₃Nb₂O₁₂ Garnet Solid-State Electrolyte Bo Dong^{†,*}, Mark P. Stockham[†], Philip A. Chater[‡], Peter R. Slater^{†,*}

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Figure S1: Simulated partial PDFs for the crystal structure of $Li_5La_3Nb_2O_{12}$. The total D(r) is shown as a dotted black line. Contributions from Nb,Ce–O, La–O, La–Nb,Ce, La–La and all other contributions (Li–Li, Li–O, Li–La, Li–Nb,Ce, O–O, Nb,Ce–Nb,Ce) are shown in red, green, yellow, purple and grey, respectively. The peak positions at approximately 2.0 Å, 2.6 Å, 3.5 Å and 4.0 Å are good indications of the local Nb,Ce–O, La–O, La–Nb,Ce and La–La bond lengths, respectively.



Figure S2: Peak fitting of PDF data to extract bond length distances (see Table 4 of main manuscript) for $Li_5La_3Nb_2O_{12}$ (top), $Li_{5.5}La_3Nb_{1.5}Ce_{0.5}O_{12}$ (middle) and $Li_{5.75}La_3Nb_{1.25}Ce_{0.75}O_{12}$ (bottom). Experimental data are shown in blue, calculated data in red and difference in grey.



Figure S3 Electrochemical impedance spectroscopy of Li//Li₅La₃Nb₂O₁₂//Li and Li//Li_{5.75}La₃Nb_{1.25}Ce_{0.75}O₁₂//Li cell.

Composition	Relative density
Li ₅ La ₃ Nb ₂ O ₁₂	51.2%
Li _{5.25} La ₃ Nb _{1.75} Ce _{0.25} O ₁₂	55.8%
Li _{5.5} La ₃ Nb _{1.5} Ce _{0.5} O ₁₂	59.1%
Li _{5.75} La ₃ Nb _{1.25} Ce _{0.75} O ₁₂	75.1%

Table S1 Relative density of Li_{5+x}La₃Nb_{2-x}Ce_xO₁₂