Electronic Supplementary Material (ESI) for RSC Advances.

Stabilization of the cubic, fast-ion conducting phase of $Li_7La_3Sn_2O_{12}$ garnet by gallium doping

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Supporting Information:

Table S1. Refined structural parameters from Rietveld fit against XRD data[a] for 0.3Ga-doped LLSO synthesized by solid-state reactions and calcined at 900 °C.

atom	site	occupation	x	y	Z	U_{iso} (Å²)
Li1[b]	24d	0.21(9)	0.375	0	0.25	0.11(1)
Ga[b]	24d	0.1	0.375	0	0.25	0.11(1)
Li2[b]	96h	0.455(25)	0.690	0.580	0.100	0.11(1)
La	24c	1	0.125	0	0.25	0.018(2)
Sn	16a	1	0	0	0	0.015(2)
O	96h	1	0.2966(7)	0.0984(8)	0.1941(3)	0.007(4)

[a] Space group $Ia\bar{3}d$, a = 12.945(3) Å; fit statistics: χ^2= 4.514; wRp = 0.1181, Rp = 0.0863.

[b] The Ga-content was fixed at 0.3 mole per unit formula of LLSO and the sum of Li1+Li2 was constrained accordingly to maintain electrical neutrality (i.e., $Li_{6.1}Ga_{0.3}La_3Sn_2O_{12}$).

Li_2SnO_3 was introduced as a second phase in the refinement (space group C2/c; lattice parameters a = 5.296(4) Å, b = 9.156(4) Å, c = 10.014(9) Å, α = 90°, β = 100.296(8)° and γ = 90°). Refined phase fraction 3.0(1) wt%.

Table S2. Refined structural parameters from Rietveld fit against XRD data[a] for 0.3Ga-doped LLSO synthesized by sol-gel method and calcined at 900 °C.

atom	site	occupation	x	y	Z	U_{iso} (Å^2)
Li1[b]	24d	0.35(14)	0.375	0	0.25	0.09(2)
Ga[b]	24d	0.095	0.375	0	0.25	0.09(2)
Li2[b]	96h	0.425(35)	0.690	0.580	0.100	0.09(2)
La	24c	1	0.125	0	0.25	0.019(1)
Sn	16a	1	0	0	0	0.015(2)
O	96h	1	0.2958(6)	0.0953(8)	0.1980(7)	0.010(4)

[a] Space group $Ia\bar{3}d$, a = 12.9522(4) Å; fit statistics: χ^2= 1.659; wRp = 0.0839, Rp = 0.0637.

[b] The Ga-content was fixed at 0.285 mole per unit formula of LLSO, as determined from ICP-MS, and the sum of Li1+Li2 was constrained accordingly to maintain electrical neutrality (i.e., $Li_{6.15}Ga_{0.285}La_3Sn_2O_{12}$).

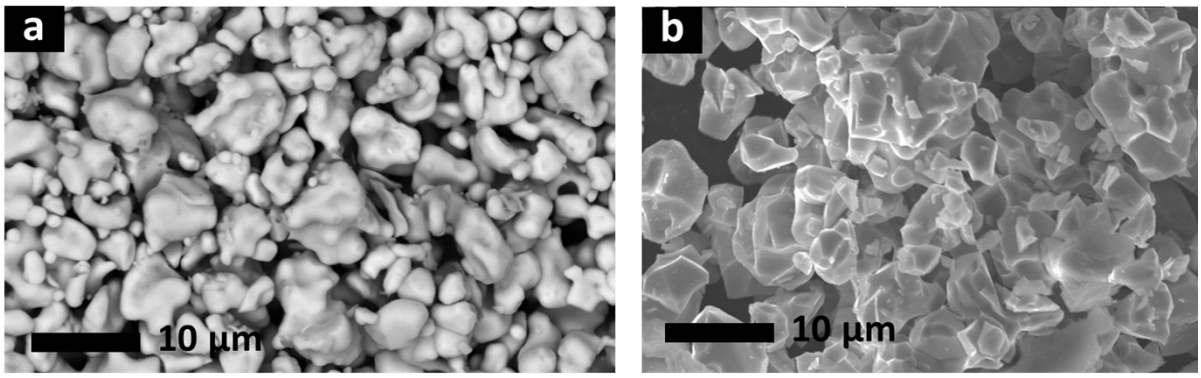

Figure S1. SEM images of 0.3Ga-doped LLSO prepared by sol-gel (a) and by solid-state reactions (b) methods.

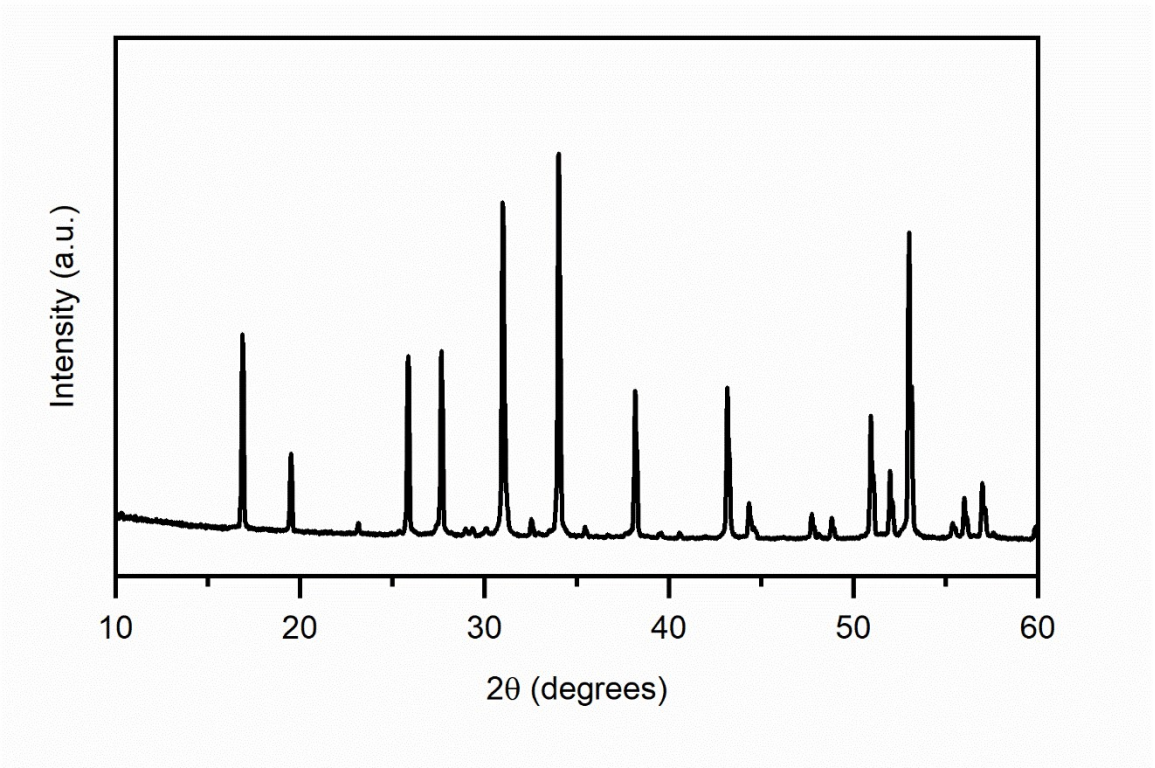

Figure S2. XRD pattern of 0.3Ga-doped LLSO synthesized by sol-gel technique and stored in air for several days.

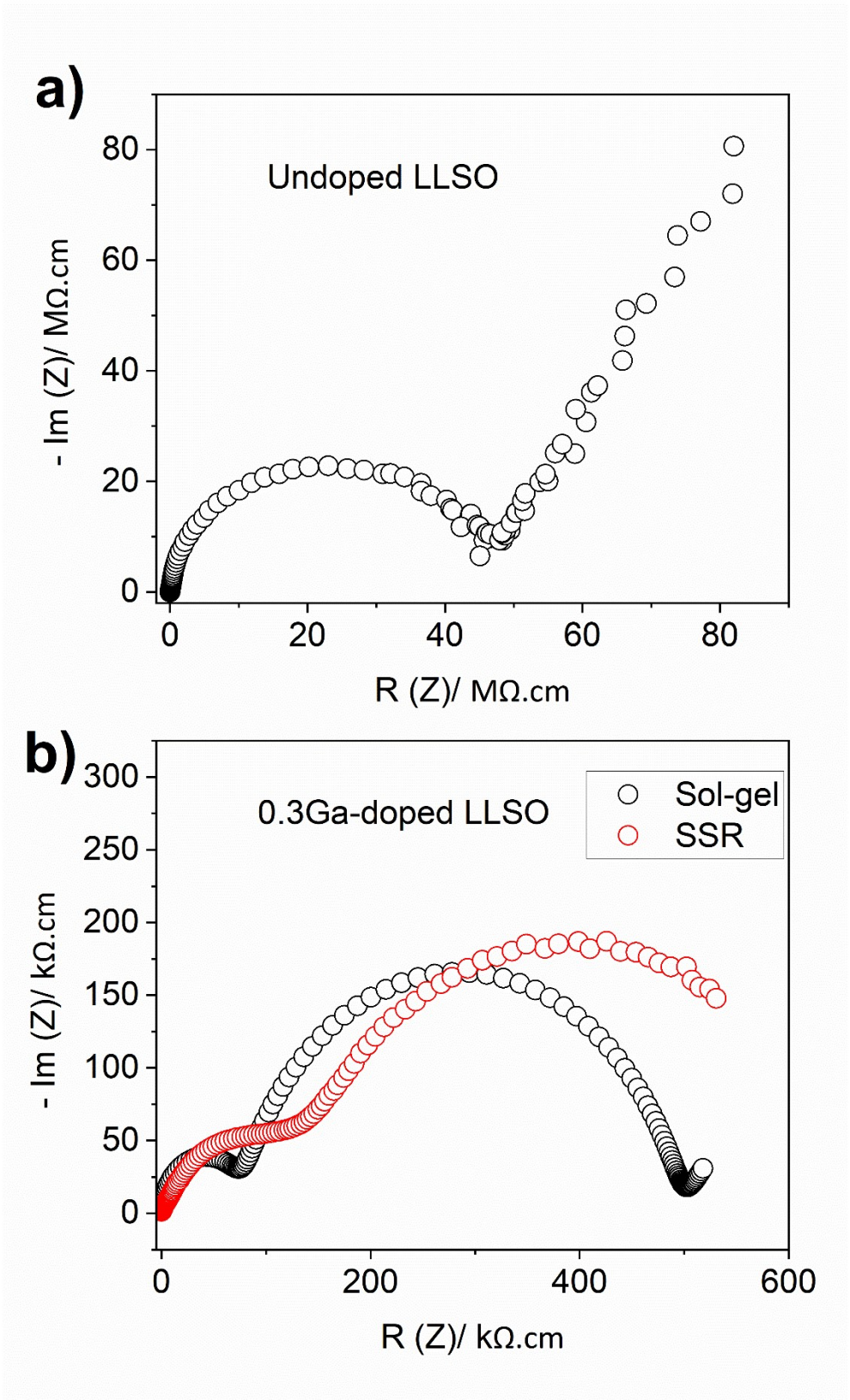

Figure S3. a) Impedance spectrum of undoped LLSO at 40 °C; total conductivity of ~ $2 \times 10^{-8} Scm^{-1}$. b) Impedance spectra of 0.3Ga-doped LLSO prepared by sol-gel and solid-state reaction (SSR) methods at 40 °C. The sample prepared by SSR showed slightly higher resistance than that prepared by sol-gel method.

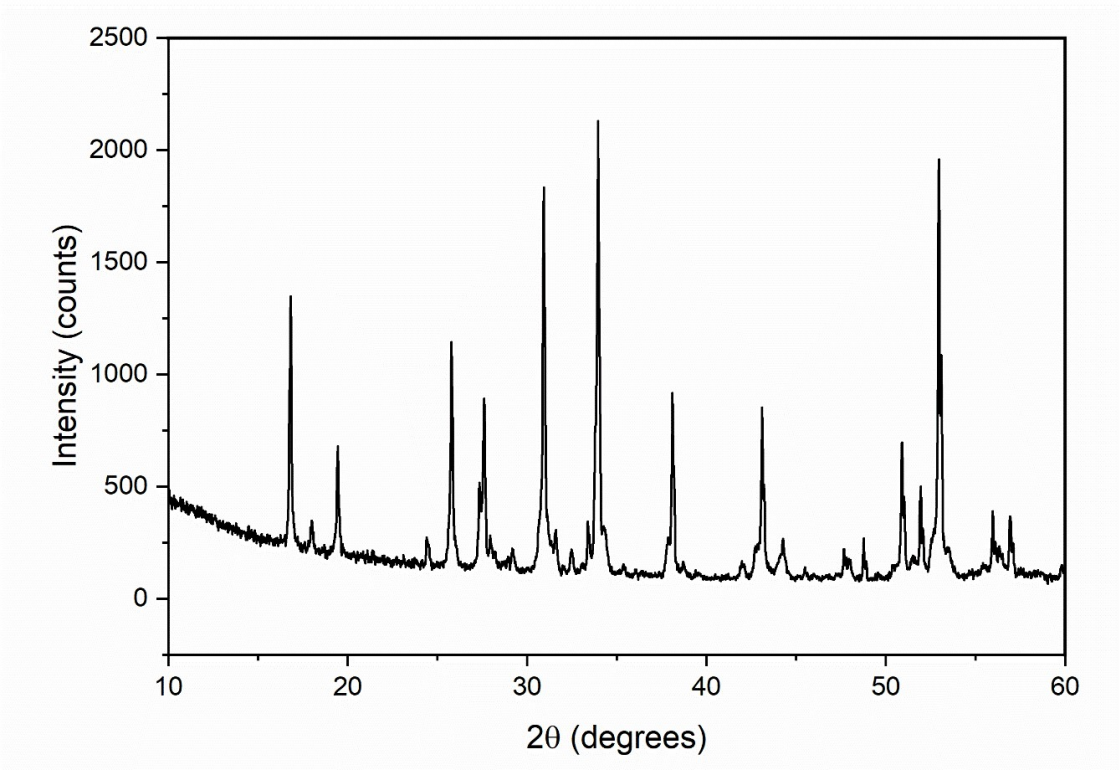

Figure S4. XRD pattern of 0.3Ga-doped LLSO synthesized by sol-gel technique and calcined at 1100^{o}C.

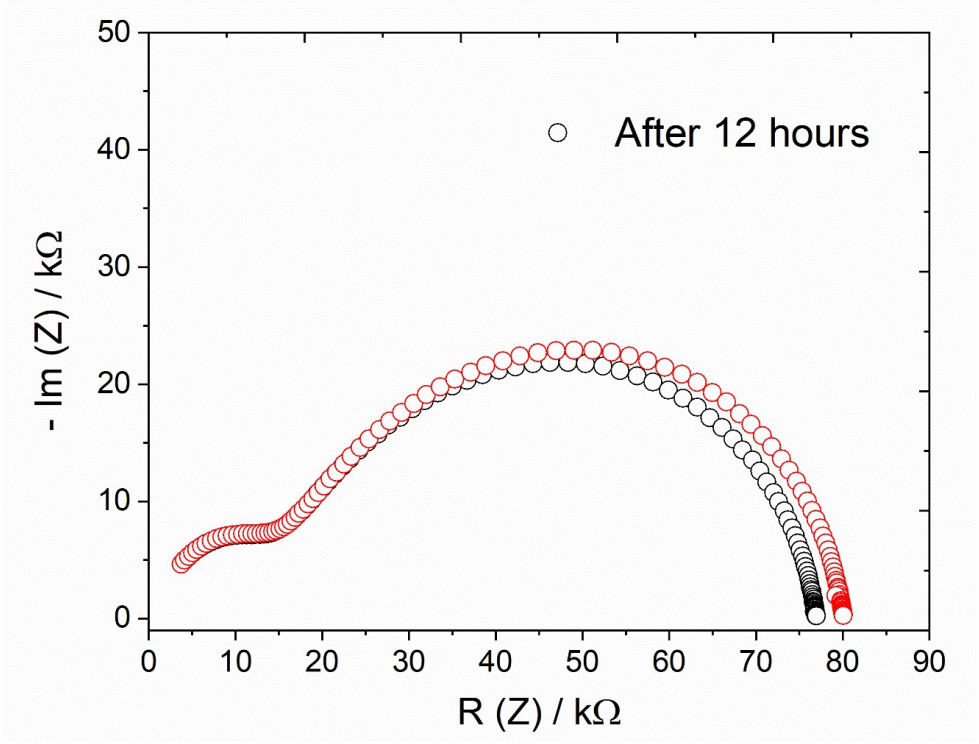

Figure S5. Impedance plots of hot-pressed 0.3Ga-doped LLSO collected at 40 °C using lithium electrodes.

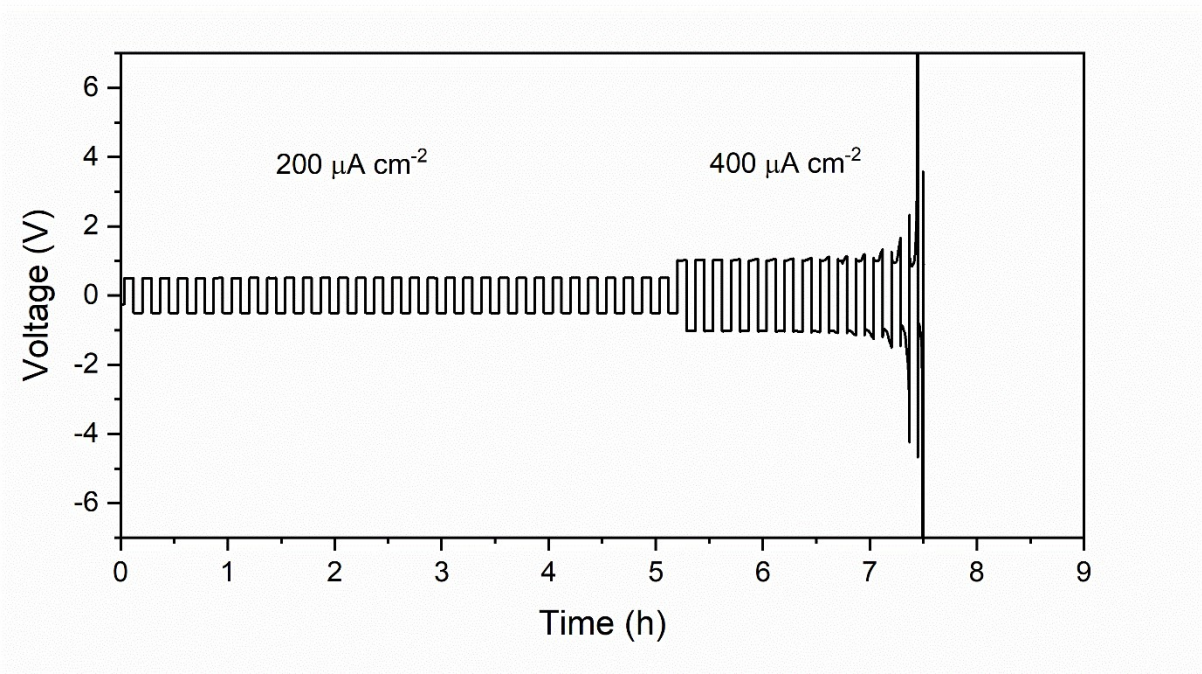

Figure S6. Galvanostatic cycling data of a Li/0.3Ga-LLSO/Li symmetric cell at 80 °C.