Supplementary information for:

Glass-like thermal conductivity in $SrTiO_3$ thermoelectrics induced by A-site vacancies

S. R. Popuri,[a] A. J. M. Scott,[a] R. A. Downie,[a] M. A. Hall,[a] E. Suard,[b] R. Decourt,[c] M. Pollet,[c] and J.-W. G. Bos[a]*

[a] *Institute of Chemical Sciences and Centre for Advanced Energy Storage and Recovery, School of engineering and physical sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom. *j.w.g.bos@hw.ac.uk*

[b] Institut Laue-Langevin, Grenoble, F-38000, France

[c] CNRS, Université de Bordeaux, ICMCB, 87 avenue du Dr. A. Schweitzer, Pessac F-33608, France

Table S1. Lattice parameters from Rietveld fits against laboratory X-ray data and pellet densities for the $Sr_{1-x}La_{0.67x}\square_{0.33x}TiO_3$, $Sr_{1-x}La_{0.67x}\square_{0.33x}Ti_{0.80}Nb_{0.20}O_{3-\delta}$ and $Sr_{0.8}La_{0.13}\square_{0.07}Ti_{1-y}Nb_yO_{3-\delta}$ series.

x	y	a (Å)	Density (%)
0	0	3.9052(1)	95(1)
0.4	0	3.8966(1)	97(1)
0.8	0	3.8843(1)	92(1)
0	0.2	3.9267(1)	92(1)
0.4	0.2	3.9056(1)	90(1)
0.8	0.2	3.8935(1)	91(1)
0.2	0	3.9082(1)	90(1)
0.2	0.05	3.9135(1)	91(1)
0.2	0.10	3.9163(1)	95(1)
0.2	0.2	3.9341(1)	93(1)

Space group Pm-3m, Sr/La/□ (0, 0, 0), Ti/Nb (1/2, 1/2, 1/2), O (1/2, 1/2, 0).

Table S2. Structural parameters for $Sr_{0.8}La_{0.13}Ti_{0.95}Nb_{0.05}O_{2.91(3)}$ from a Rietveld fit against super-D2B neutron powder diffraction data.

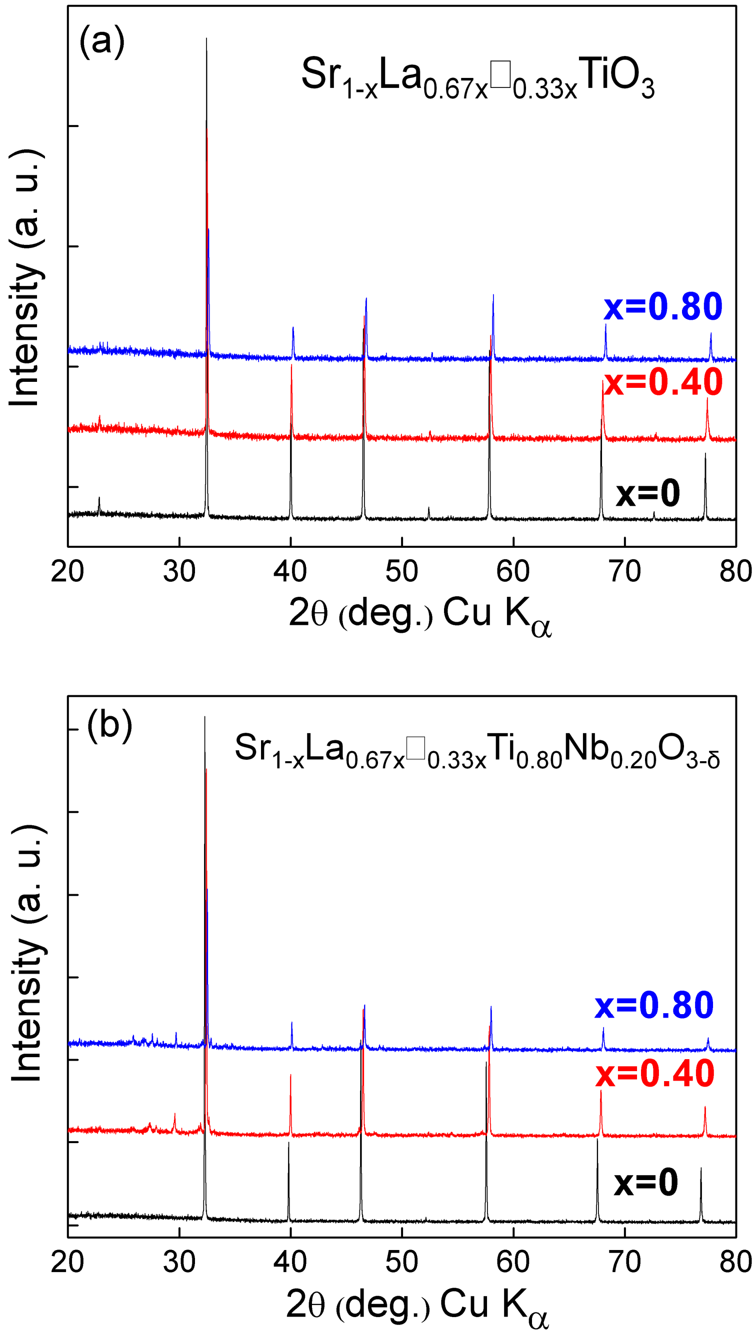
	Wyckoff	**x**	**y**	**z**	**Occupancy**	**U_{iso} ($Å^2$)**
Sr/ La	4b	0	0.5	0.25	0.798(3)/ 0.130(3)	0.006(1)
Ti/ Nb	4c	0	0	0	0.95/ 0.05	0.005(1)
O1	4a	0	0	0.25	0.96(5)	0.012(1)
O2	8h	0.2381(2)	0.7381(2)	0.5	0.97(2)	0.006(1)

Space Group I4/mcm; a = 5.5327(1) Å; c = 7.8324(4) Å.

Table S3. Selected bond distances (Å) and angles (°) for $Sr_{0.8}La_{0.13}Ti_{0.95}Nb_{0.05}O_{2.91(3)}$.

	Distance/ Angle
Ti/Nb-O1 (×2)	1.95809(9)
Ti/Nb-O2 (×4)	1.95831(9)
Ti/Nb-O1-Ti/Nb	180
Ti/Nb-O2-Ti/Nb	174.57(9)
Sr/La-O1 (×4)	2.76635(7)
Sr/La-O2 (×4)	2.7030(10)
Sr/La-O2 (×4)	2.8341(11)

Fig. S1. Room temperature powder X-ray diffraction patterns for the (a) $Sr_{1-x}La_{0.67x}\square_{0.33x}O_3$, (b) $Sr_{1-x}La_{0.67x}\square_{0.33x}Ti_{0.8}Nb_{0.2}O_{3-\delta}$ and (c) $Sr_{0.80}La_{0.13}\square_{0.07}Ti_{1-y}Nb_yO_{3-\delta}$ series.



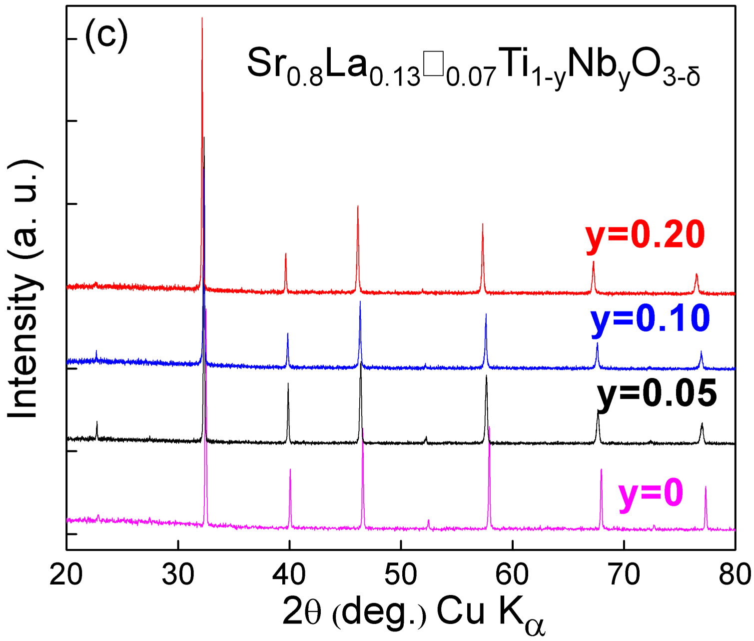

(c)
Sr0.8La0.13□0.07Ti1-yNbyO3-δ
y=0.20
y=0.10
y=0.05
y=0
Intensity (a. u.)
20
30
40
50
60
70
80
2θ (deg.) Cu Kα

Fig. S2. Temperature dependence of the thermal diffusivity (α) and specific heat (C_p) for the $Sr_{1-x}La_{0.67x}\square_{0.33}TiO_3$ series.

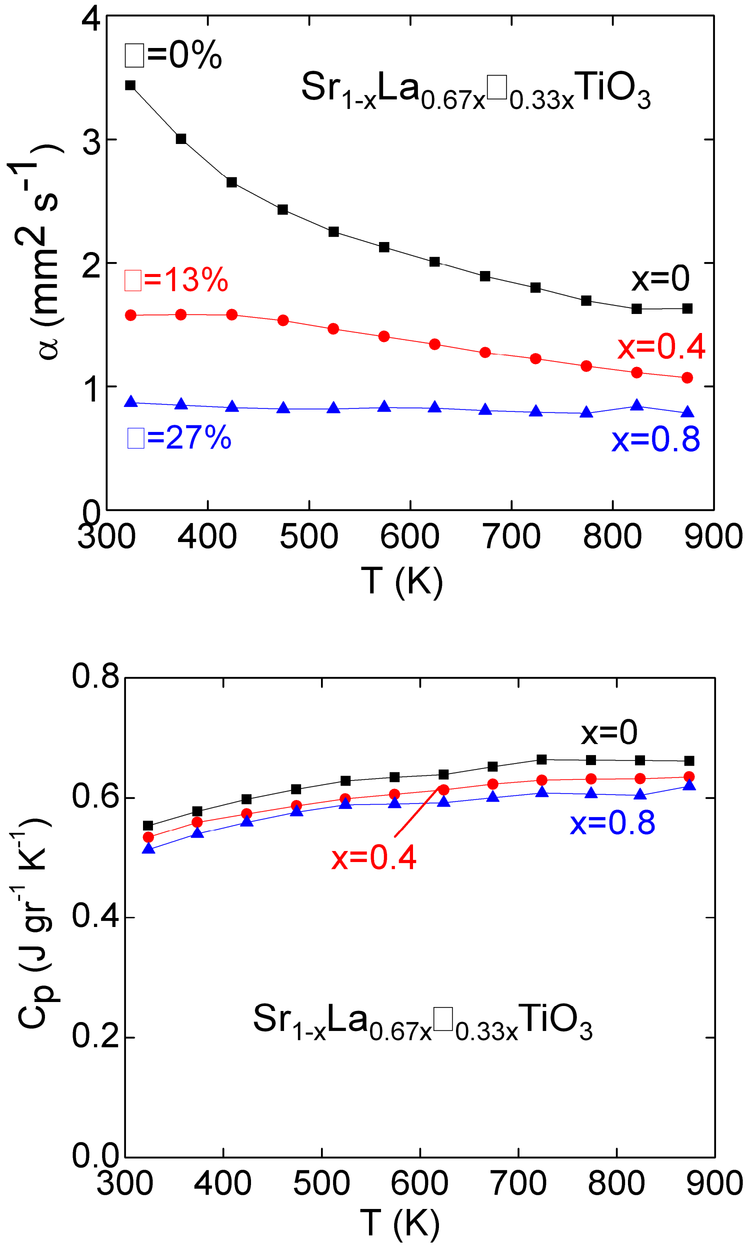


Fig. S3. Temperature dependence of the Seebeck coeffient (S) and electrical resistivity (ρ) for the $Sr_{1-x}La_{0.67x}\square_{0.33}Ti_{0.8}Nb_{0.2}O_3$ series.

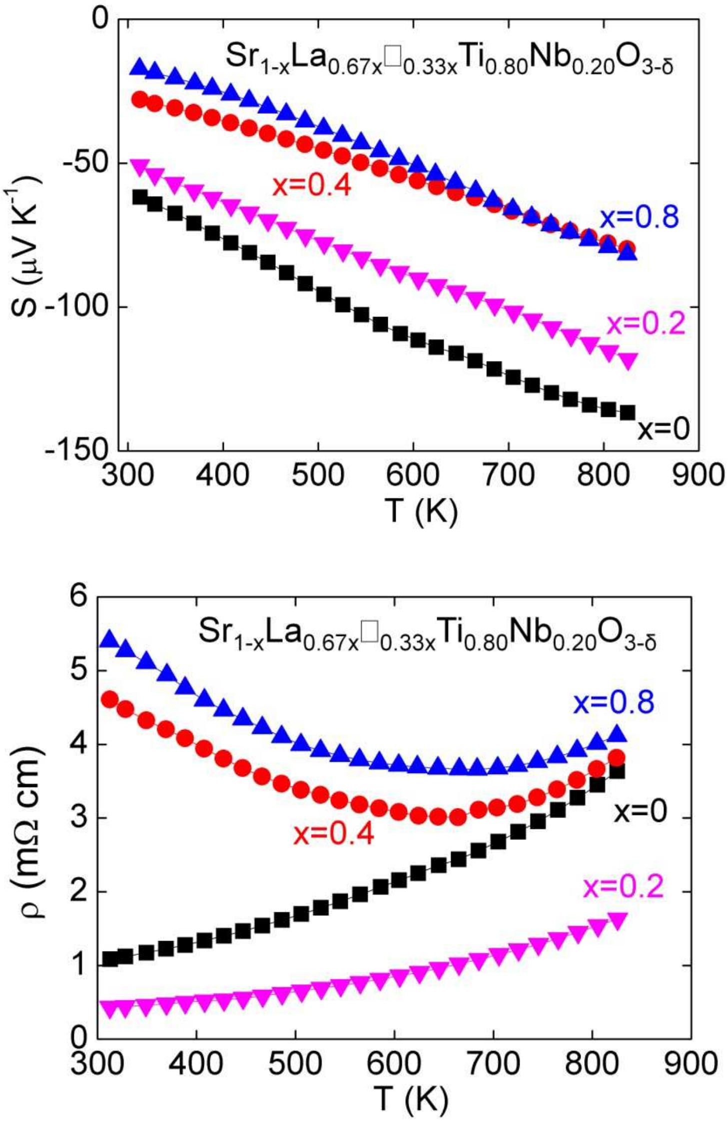


Fig. S4. Observed (circles), calculated (solid line) and difference Rietveld neutron diffraction profiles for $Sr_{0.80}La_{0.13}\square_{0.07}Ti_{0.95}Nb_{0.05}O_{2.91(3)}$. The bottom row of Bragg markers is for a 1.0(2) wt% TiO_2 impurity. Fit statistics: χ^2 = 4.1, wR_p = 4.0%, R_p = 3.2%, R_F^2 = 2.2%.