

SUPPLEMENTARY INFORMATION

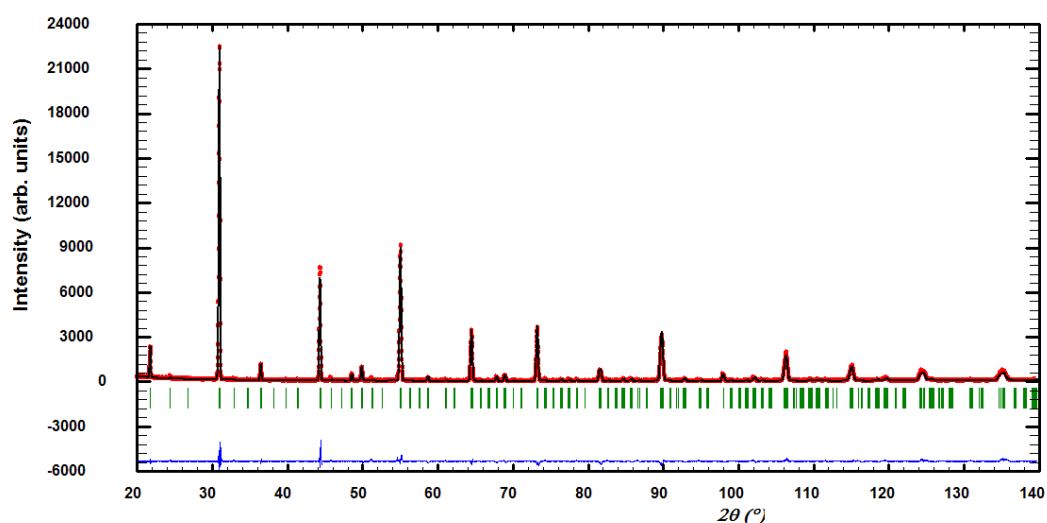


Figure SI 1: Experimental (red circles) and calculated (black continuous line) XRD patterns (and their difference, blue line at the bottom) for $\text{Sr}_2\text{LuNb}_{0.90}\text{Ti}_{0.10}\text{O}_6$ assuming S.G. $P2_1/n$. The green vertical bars indicate the positions of the Bragg peaks.

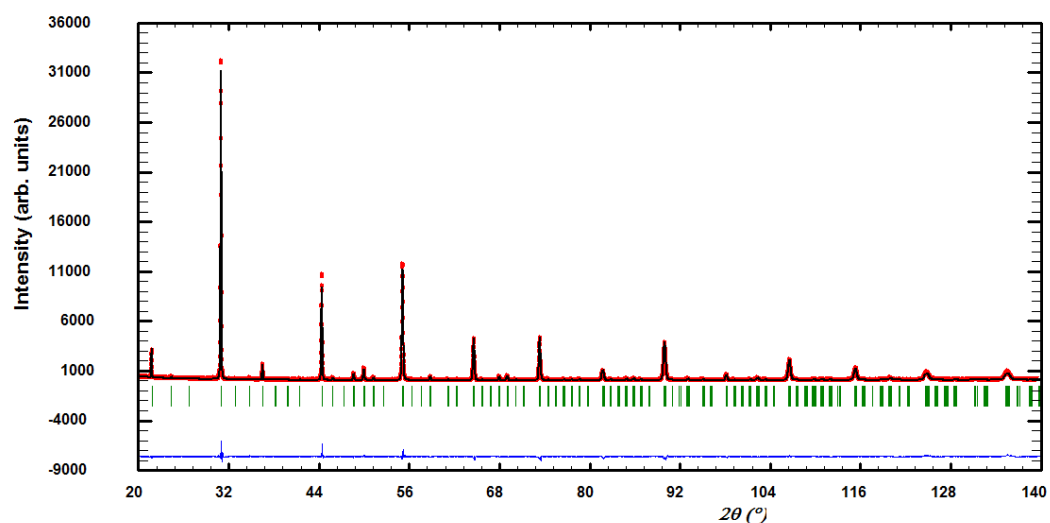


Figure SI 2: Experimental (red circles) and calculated (black continuous line) XRD patterns (and their difference, blue line at the bottom) for $\text{Sr}_2\text{LuNb}_{0.80}\text{Ti}_{0.20}\text{O}_6$ assuming S.G. $P2_1/n$. The green vertical bars indicate the positions of the Bragg peaks.

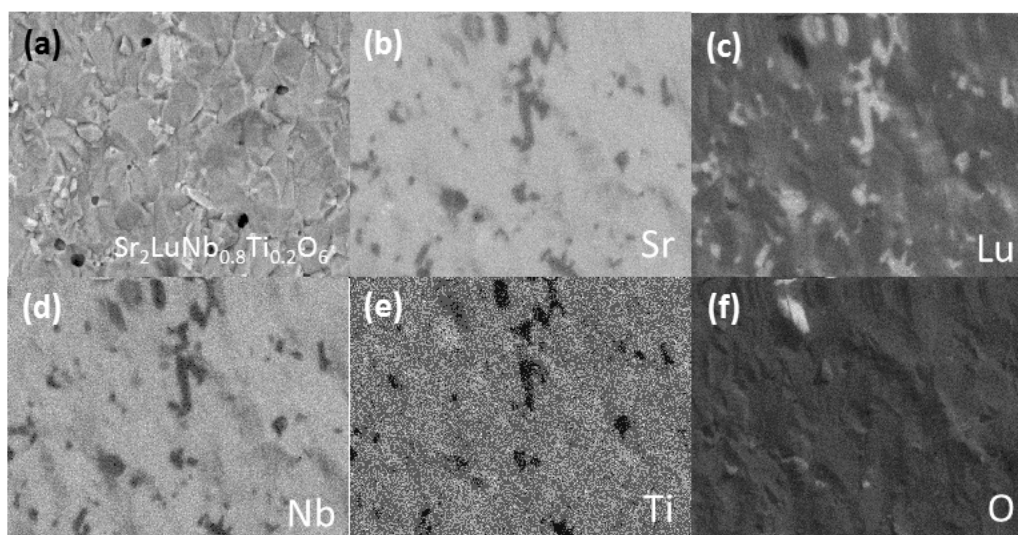


Figure SI 3: (a) Back-scattered electrons (BSE) image taken at a magnification of x 2000 and element-distribution maps of $\text{Sr}_2\text{LuNb}_{0.8}\text{Ti}_{0.2}\text{O}_6$ sample: (b) Sr, (c) Lu, (d) Nb, (e) Ti and (f) O.

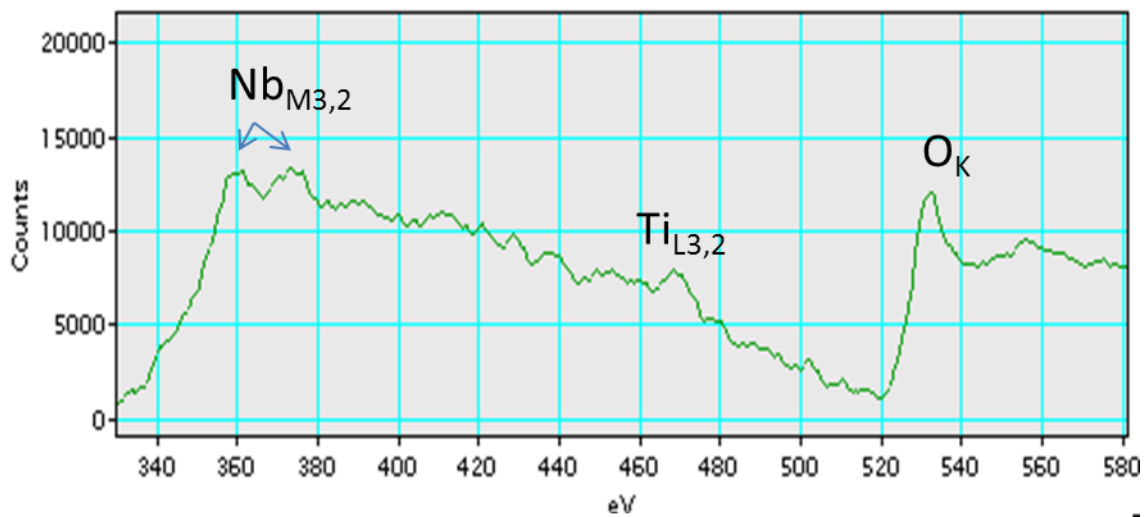


Figure SI 4: EELS spectra of the Nb $M_{3,2}$, Ti $L_{3,2}$, O K edges for $Sr_2LuNb_{0.9}Ti_{0.1}O_6$.

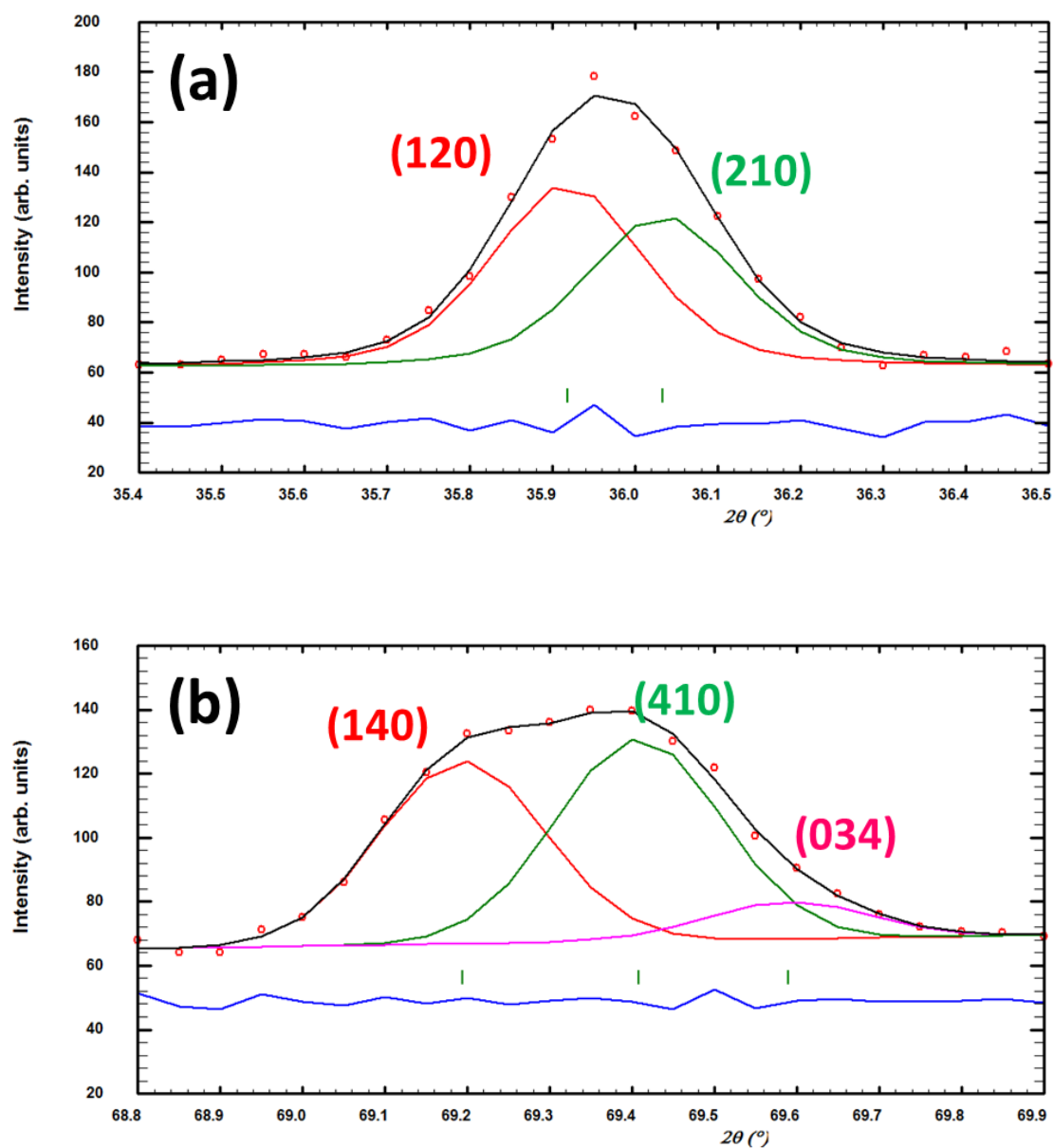


Figure SI 5: Enlarged plot of the NPD zone where Bragg peaks (a) (120)/(210) and (b) (140)/(410) appear. These maxima are not compatible with S.G. P2nn previously proposed for $\text{Sr}_2\text{LuNbO}_6$ (Sirotkin, V.P., Efremov, V.A., Trunov, V K.; The crystal structures of $\text{Sr}_2\text{SmNbO}_6$ and $\text{Sr}_2\text{TmNbO}_6$, *Russian Journal of Inorganic Chemistry* **1985**, 30(7), 981-983).

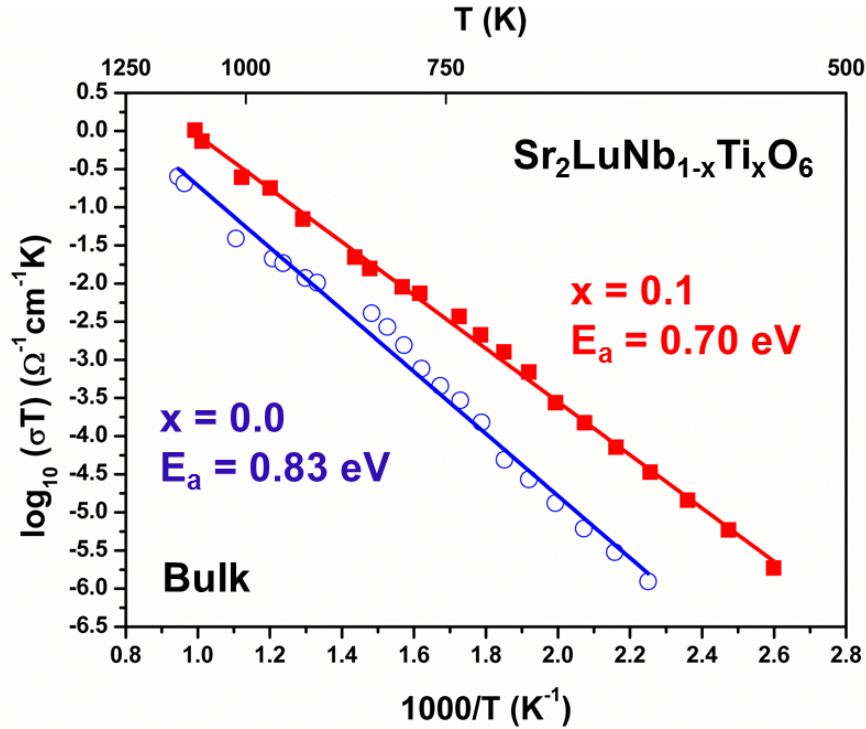


Figure SI 6: Arrhenius plots showing the temperature dependence of the bulk conductivity of Sr₂LuNb_{1-x}Ti_xO₆ (x=0 and 0.1). Activation energies are also indicated.

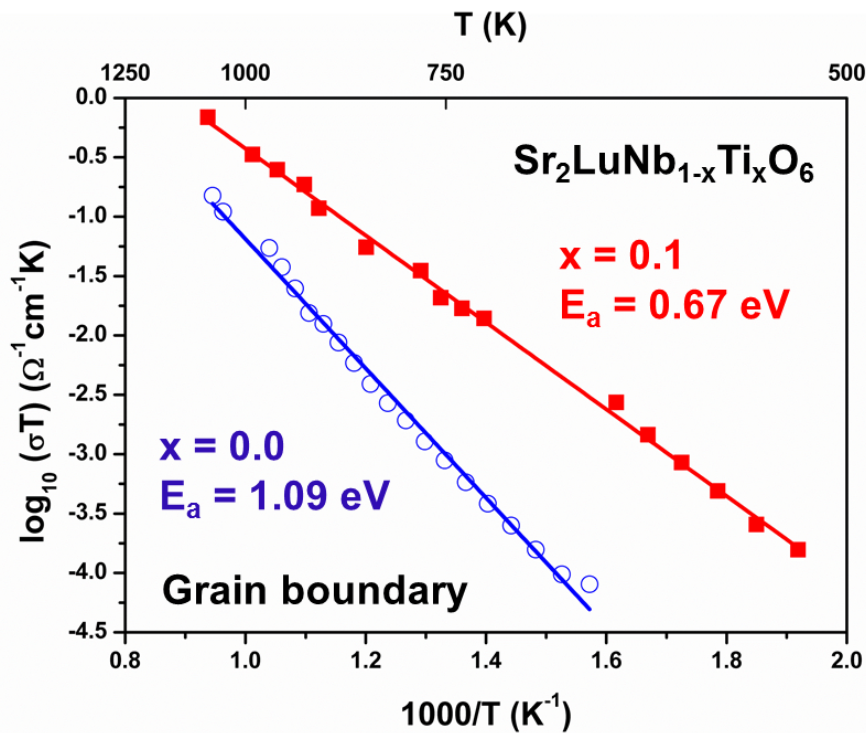


Figure SI 7: Arrhenius plots showing the temperature dependence of the grain boundary conductivity of Sr₂LuNb_{1-x}Ti_xO₆ (x=0 and 0.1). Activation energies are also indicated.

Table SI1: Structural parameters for Sr₂LuNb_{1-x}Ti_xO₆ compounds obtained from XRD.

	^b Sr ₂ LuNbO ₆	^c Sr ₂ LuNb _{0.90} Ti _{0.10} O ₆	^d Sr ₂ LuNb _{0.80} Ti _{0.20} O ₆
Space Group^a	P2 ₁ /n	P2 ₁ /n	P2 ₁ /n
a (Å)	5.7951(2)	5.7845(2)	5.7596(2)
b (Å)	5.7974(2)	5.7666(2)	5.7732(1)
c (Å)	8.1989(3)	8.1618(3)	8.1521(3)
β (deg)	90.221(2)	90.048(2)	90.056(3)
Sr position	4e	4e	4e
X	-0.0023(7)	0.0010(7)	-0.0054(6)
y	0.0202(3)	0.0166(3)	0.0200(2)
Z	0.7510(7)	0.7479(6)	0.7492(6)
U*100 (Å²)	1.52(6)	0.95(4)	0.64(3)
B' position	2c	2c	2c
Occ Nb/Ti	0.50/0.00	0.449(3)/0.051(3)	0.404(3)/0.096(3)
U*100 (Å²)	0.84(4)	0.18(5)	0.47(4)
B'' position	2d	2d	2d
Occ Lu	0.50	0.50	0.50
U*100 (Å²)	0.86(4)	0.22(4)	0.12(4)
O(1) position	4e	4e	4e
X	0.276(4)	0.316(4)	0.319(3)
y	0.320(4)	0.337(4)	0.329(2)
Z	0.970(2)	0.948(3)	0.950(2)
Occ	1.00	1.00	1.000(1)
U*100 (Å²)	1.76(6)	0.81(4)	0.46(3)
O(2) position	4e	4e	4e
X	0.289(4)	0.291(4)	0.281(3)
y	0.272(3)	0.268(4)	0.264(3)
Z	0.549(3)	0.550(3)	0.531(2)
Occ	1.00	1.00	1.000(1)
U*100 (Å²)	1.76(6)	0.81(4)	0.46(3)
O(3) position	4e	4e	4e
X	0.931(4)	0.003(4)	0.968(4)
y	0.486(2)	0.491(2)	0.495(1)
Z	0.756(2)	0.755(2)	0.747(2)
Occ	1.00	1.00	1.000(1)
U*100 (Å²)	1.76(6)	0.81(4)	0.46(3)

^a P2₁/n: 2c (0 ½ 0), 2d (½ 0 0), 4e (xyz)

^b χ²= 3.47, R_{wp}= 13.1%, R_{exp}= 7.01%, R_B= 4.45%, Composition: Sr₂LuNbO₆

^c χ²= 3.85, R_{wp}= 12.9%, R_{exp}= 6.55%, R_B= 6.63%, Composition: Sr₂LuNb_{0.898(2)}Ti_{0.102(2)}O₆

^d χ²= 2.33, R_{wp}= 9.63%, R_{exp}= 6.31%, R_B= 4.62%, Composition: Sr₂LuNb_{0.808(2)}Ti_{0.192(2)}O₆

Table S12: Selected structural information for $\text{Sr}_2\text{LuNb}_{1-x}\text{Ti}_x\text{O}_6$ compounds obtained from XRD data. Angles are given in degrees and distances in Å.

	$\text{Sr}_2\text{LuNbO}_6$	$\text{Sr}_2\text{LuNb}_{0.90}\text{Ti}_{0.10}\text{O}_6$	$\text{Sr}_2\text{LuNb}_{0.80}\text{Ti}_{0.20}\text{O}_6$
B'-O(1) x 2	1.92(2)	2.10(2)	2.12(2)
B'-O(2) x 2	2.04(2)	1.98(2)	2.00(2)
B'-O(3) x 2	2.04(2)	2.00(2)	1.99(2)
Average B'-O	1.997(8)	2.025(9)	2.035(7)
Distortion B'-O₆ x 10⁴	8.442	6.897	9.078
B''-O(1) x 2	2.29(2)	2.26(2)	2.21(1)
B''-O(2) x 2	2.17(2)	2.21(2)	2.13(2)
B''-O(3) x 2	2.14(2)	2.10(2)	2.10(2)
Average B''-O	2.200(8)	2.182(9)	2.148(6)