

Electronic Supplemental Information:

Resilience of the Aurivillius structure upon La and Cr doping in
 $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$ multiferroic.

Omar Alejandro Salas, Yohannes W. Getahun, Cein H. Mandujano, Felicia Manciu,
Mariana Castellanos, Jorge Lopez, Raquel Garza Hernandez, Volodymir B. Buturlim,
Krzysztof Gofryk, Dhanpal Bairwa, Suja Elizabeth, Harikrishnan S. Nair.

BTFO	x	y	z	Occupancy	U_{iso}
Bi1 4a	0.2511	0.2474	0	1	0.0153
Bi2 8b	0.2452	0.2449	0.1047	1	0.0095
Bi3 8b	0.2294	0.2709	0.1044	1	0.0106
Ti1 8b	0.2951	0.2505	0.4507	0.75	0.0072
Fe1 8b	0.2951	0.2505	0.4507	0.25	0.0072
Ti2 8b	0.2814	0.2501	0.3471	0.75	0.0064
Fe2 8b	0.2814	0.2501	0.3471	0.25	0.0064
O1 4a	0.3208	0.1754	0.5	1	0.0012
O2 8b	0.6056	0.5439	0.0533	1	0.0195
O3 8b	0.3338	0.3072	0.4048	1	0.0076
O4 8b	0.5316	0.4940	0.1385	1	0.0153
O5 8b	0.2974	0.2047	0.3075	1	0.0171
O6 8b	0.5206	0.5004	0.2538	1	0.0082
O7 8b	0.0342	-0.0343	0.0392	1	0.0299
O8 8b	0.0989	0.0203	0.1456	1	0.0087

Table S1. The Rietveld-refined atomic parameters of BTFO in the spacegroup $A2_1am$. Occupancies were fixed to nominal stoichiometry.

BLTFO	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	U_{iso}
Bi1 4 <i>a</i>	0.2732	0.2521	0	1	0.0156
Bi2 8 <i>b</i>	0.2831	0.2403	0.1048	1	0.0081
Bi3 8 <i>b</i>	0.2539	0.2709	0.2196	1	0.0106
Ti1 8 <i>b</i>	0.2773	0.2571	0.4511	0.75	0.0063
Fe1 8 <i>b</i>	0.2692	0.2693	0.4490	0.25	0.0063
Ti2 8 <i>b</i>	0.2337	0.2552	0.3444	0.75	0.0063
Fe2 8 <i>b</i>	0.2297	0.2639	0.3435	0.25	0.0063
O1 4 <i>a</i>	0.3033	0.2227	0.5	1	0.0012
O2 8 <i>b</i>	0.5407	0.6016	0.0498	1	0.008
O3 8 <i>b</i>	0.3121	0.2887	0.4107	1	0.0146
O4 8 <i>b</i>	0.5198	0.4356	0.1349	1	0.0018
O5 8 <i>b</i>	0.3425	0.2194	0.3113	1	0.0322
O6 8 <i>b</i>	0.4909	0.4765	0.2561	1	0.0093
O7 8 <i>b</i>	0.0474	0.0202	0.0403	1	0.0188
O8 8 <i>b</i>	0.0426	-0.0902	0.1448	1	0.0248
La1 4 <i>a</i>	0.2732	0.2521	0	1	0.0156
La2 8 <i>b</i>	0.2831	0.2403	0.1048	1	0.0081
La3 8 <i>b</i>	0.2539	0.2709	0.2196	1	0.0106

Table S2. The Rietveld-refined atomic parameters of BLTFO in the spacegroup $A2_1am$. Occupancies were fixed to nominal stoichiometry.

BTFCO	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	U_{iso}
Bi1 4 <i>a</i>	0.2470	0.2656	0	1	0.0139
Bi2 8 <i>b</i>	0.2420	0.2367	0.1039	1	0.0092
Bi3 8 <i>b</i>	0.2285	0.2459	0.2188	1	0.012
Ti1 8 <i>b</i>	0.2893	0.2458	0.4502	0.75	0.012
Fe1 8 <i>b</i>	0.2893	0.2458	0.4502	0.125	0.012
Ti2 8 <i>b</i>	0.2920	0.2283	0.3468	0.75	0.012
Fe2 8 <i>b</i>	0.2920	0.2283	0.3468	0.25	0.012
O1 4 <i>a</i>	0.3236	0.1951	0.5	1	0.0012
O2 8 <i>b</i>	0.5817	0.5529	0.0502	1	0.012
O3 8 <i>b</i>	0.3584	0.3047	0.4055	1	0.0278
O4 8 <i>b</i>	0.5429	0.5053	0.1349	1	0.0407
O5 8 <i>b</i>	0.3034	0.2194	0.3055	1	0.0273
O6 8 <i>b</i>	0.5528	0.4818	0.2551	1	0.0120
O7 8 <i>b</i>	-0.0239	-0.0613	0.0393	1	0.0111
O8 8 <i>b</i>	0.0849	-0.0182	0.1494	1	0.0420
Cr1 8 <i>b</i>	0.2893	0.2458	0.4502	0.125	0.010
Cr2 8 <i>b</i>	0.2920	0.2283	0.3468	0.125	0.010

Table S3. The Rietveld-refined atomic parameters of BTFCO in the spacegroup $A2_1am$. Occupancies were fixed to nominal stoichiometry.

	BTFO	BTFCO	BLTFO
Bi1-Bi1	3.853(7)	3.83(3)	3.833(3)
Bi1-Bi2	4.3142(8)	4.2721(17)	4.3273(8)
Bi1-O1	2.31(3), 2.38(3)	2.292(15), 2.379(12)	2.48(4), 2.46(4)
Bi1-O2	2.45(3)	2.438(8)	2.52(3)
Bi1-O7	2.48(3)	2.473(10)	2.43(3)
Ti1/Fe1-O1	2.030(7)	2.01926(8)	2.068(8)
Ti1/Fe1-O2	1.99(3)	1.86126(12)	1.90(3)
Ti1/Fe1-O3	2.035(14)	2.02279(9)	1.892(13)
Ti1/Fe1-O7	2.28(4)	2.27987(3)	2.24(4)
∠ Ti1-O7-Ti1	153.8(13)	153.8833(11)	154.2(12)
∠ Ti1-O3-Ti2	156.1(13)	155.9009(12)	154.4(12)
∠ Ti2-O8-Ti2	169.1(13)	169.2103(8)	157.7(13)

Table S4. Selected bond parameters of BTFO, BTFCO and BLTFO obtained from the Rietveld refinement of synchrotron X-ray diffraction data. The distances are in the units of Å and the angles are in degrees.