Novel multiferroic state and magnetoelectric enhancement by breaking the geometric magnetic frustration in $LuMn_{1-x}O_3$

F. G. Figueiras [1, 2, *], D. Karpinsky [1, 3, 4], P. B. Tavares [5], J. N. Gonçalves [1], S. Yañez-Vilar [2], A. F. Moreira Dos Santos [6], A. Franz [7], M. Tovar [7], J. Agostinho Moreira [2], . S. Amaral [1]

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Supplementary Information

Table 1: $LuMn_{0.98}O_3$ crystallographic parameters and Rietveld refinement quality factors calculated from NPD results

T (K)	*S. G.*	*a*, *b* (Å)	*a*, *b* ***Error*** (Å)	*c* (Å)	*c* ***Error*** (Å)	**Vol.** cell Z = 6 (Å³)	***density*** *(calc.)*	χ^2	R_p
2	$P6_3cm$ (185)	6.0280	$\pm1*10^{-4}$	11.3618	$\pm2*10^{-4}$	357.534	7.714	2.18	4.69
10	$P6_3cm$ (185)	6.0301	$\pm1*10^{-4}$	11.3672	$\pm2*10^{-4}$	357.959	7.704	2.59	7.46
50	$P6_3cm$ (185)	6.0299	$\pm1*10^{-4}$	11.3656	$\pm2*10^{-4}$	357.885	7.706	2.38	8.31
80	$P6_3cm$ (185)	6.0317	$\pm1*10^{-4}$	11.3650	$\pm2*10^{-4}$	358.080	7.702	2.39	9.60
100	$P6_3cm$ (185)	6.0329	$\pm1*10^{-4}$	11.3648	$\pm2*10^{-4}$	358.216	7.699	2.42	11.1
300	$P6_3cm$ (185)	6.0448	$\pm1*10^{-4}$	11.3653	$\pm2*10^{-4}$	359.646	7.668	2.55	10.4

Table 2: $LuMn_{0.98}O_3$ unit cell bond and angle between Mn and O ions.

T (K)	**Mn-O1** (Å) #10	**Mn-O2** (Å) #10	**Mn-O3** (Å) #10	**Mn-O4** (Å) #12	**<Mn-O>** (Å) #22	**Mn-O3-Mn** (º) #2	**Mn-O4-Mn** (º) #12	**O1-Mn-O2** (º) #6	**<Mn-Mn>** (Å) *NN #3*	**<Mn-Mn>** (Å) *NNN #2*
2	1.892	1.852	1.924	2.079	2.009	117.92	118.61	172.67	3.530	6.046
10	1.862	1.822	2.109	1.979	2.038	118.24	119.20	175.04	3.563	6.016
50	1.785	1.835	2.126	1.977	2.045	116.09	119.80	176.11	3.567	6.017
80	1.767	1.882	2.134	1.976	2.048	115.48	119.84	176.52	3.575	6.016
100	1.828	1.859	2.140	1.975	2.050	115.95	119.55	175.52	3.585	6.015
300	1.828	1.884	2.078	2.011	2.041	116.32	119.28	179.49	3.576	6.026

Table 3: $LuMn_{0.98}O_3$ hexagonal unit cell magnetic moment projections and basal polarization calculated from NPD results

T (K)	$\langle\mu\rangle/_{Mn}$ (μ_B)	$\Sigma\mu_x$ (μ_B)	$\Sigma\mu_y$ (μ_B)	$\Sigma\mu_z$ (μ_B)	$\lvert\mu\rvert/_{cell}$ (μ_B)	$P_x(\mu_i)$ $*K_\mu$	$P_y(\mu_i)$ $*K_\mu$	$\lvert P_{xy}\rvert(\mu_i)$ $*K_x(\mu)$
2	2.84 ±8%	-2.301	-1.351	0.613	2.094	23.92	-5.33	24.50
10	2.7 ±8%	-1.984	-1.136	0.724	1.778	26.21	-1.72	26.27
50	2.1 ±8%	-2.981	-1.343	0.065	1.913	17.58	-0.05	17.58
80	1.9 ±8%	-2.536	-1.219	0.911	1.591	27.45	-0.80	27.46
100	n. a.	0	0	0	0	0	0	0
300	n. a.	0	0	0	0	0	0	0

Table 4: $LuMn_{0.98}O_3$ hexagonal unit cell atomic positions and Mn ions magnetic moments calculated from NPD results

T (K)	atom	Z	site	*x*	*y*	*z*
2	Lu1	71	2a	0.0000	0.0000	0.2779
	Lu2	71	4b	0.3333	0.6667	0.2345
	Mn	25	6c	0.3157	0.0000	0.0000
	O1	8	6c	0.3087	0.0000	0.1665
	O2	8	6c	0.6383	0.0000	0.3388
	O3	8	2a	0.0000	0.0000	0.4754
	O4	8	4b	0.3333	0.6667	0.0217

atom	*x*	*y*	*z*	μ_x (μ_B)	μ_y (μ_B)	μ_z (μ_B)
Mn1	0.316	0	0	-2.704	-2.956	0.098
Mn2	0	0.316	0	-0.011	-2.844	0.100
Mn3	0.666	0.666	0	2.367	3.146	0.107
Mn4	0.316	0.316	0.5	-1.952	1.304	0.108
Mn5	0.666	0	0.5	1.233	-2.013	0.100
Mn6	0	0.666	0.5	-1.235	2.012	0.100

T (K)	atom	Z	site	*x*	*y*	*z*
10	Lu1	71	2a	0.0000	0.0000	0.2684
	Lu2	71	4b	0.3333	0.6667	0.2298
	Mn	25	6c	0.3466	0.0000	0.0000
	O1	8	6c	0.3065	0.0000	0.1624
	O2	8	6c	0.6402	0.0000	0.3399
	O3	8	2a	0.0000	0.0000	0.4652
	O4	8	4b	0.3333	0.6667	0.0156

atom	*x*	*y*	*z*	μ_x (μ_B)	μ_y (μ_B)	μ_z (μ_B)
Mn1	0.344	0	0	-2.191	-3.200	0.193
Mn2	0	0.344	0	-0.639	-3.103	0.104
Mn3	0.656	0.656	0	2.147	3.215	0.151
Mn4	0.344	0.344	0.5	-1.330	1.927	0.145
Mn5	0.656	0	0.5	1.076	-2.143	0.102
Mn6	0	0.656	0.5	-1.046	2.168	0.029

T (K)	atom	Z	site	*x*	*y*	*z*
50	Lu1	71	2a	0.0000	0.0000	0.2629
	Lu2	71	4b	0.3333	0.6667	0.2209
	Mn	25	6c	0.3455	0.0000	0.0000
	O1	8	6c	0.3098	0.0000	0.1559
	O2	8	6c	0.6384	0.0000	0.3333
	O3	8	2a	0.0000	0.0000	0.4625
	O4	8	4b	0.3333	0.6667	0.0077

atom	*x*	*y*	*z*	μ_x (μ_B)	μ_y (μ_B)	μ_z (μ_B)
Mn1	0.344	0	0	-1.767	-3.276	0.004
Mn2	0	0.344	0	-1.446	-3.272	0.009
Mn3	0.656	0.656	0	1.580	3.279	0.003
Mn4	0.344	0.344	0.5	-1.075	2.146	0.002
Mn5	0.656	0	0.5	0.936	-2.254	0.017
Mn6	0	0.656	0.5	-1.210	2.034	0.030

T (K)	atom	Z	site	*x*	*y*	*z*
80	Lu1	71	2a	0.0000	0.0000	0.2613
	Lu2	71	4b	0.3333	0.6667	0.2208
	Mn	25	6c	0.3455	0.0000	0.0000
	O1	8	6c	0.3094	0.0000	0.1543
	O2	8	6c	0.6349	0.0000	0.3347
	O3	8	2a	0.0000	0.0000	0.4595
	O4	8	4b	0.3333	0.6667	0.0070

atom	*x*	*y*	*z*	μ_x (μ_B)	μ_y (μ_B)	μ_z (μ_B)
Mn1	0.344	0	0	-2.207	-3.186	0.273
Mn2	0	0.344	0	-0.766	-3.142	0.124
Mn3	0.656	0.656	0	1.852	3.261	0.200
Mn4	0.344	0.344	0.5	-1.450	1.817	0.158
Mn5	0.656	0	0.5	1.076	-2.142	0.120
Mn6	0	0.656	0.5	-1.041	2.173	0.035

T (K)	atom	Z	site	*x*	*y*	*z*
100	Lu1	71	2a	0.0000	0.0000	0.2662
	Lu2	71	4b	0.3333	0.6667	0.2264
	Mn	25	6c	0.3473	0.0000	0.0000
	O1	8	6c	0.3087	0.0000	0.1595
	O2	8	6c	0.6374	0.0000	0.3366
	O3	8	2a	0.0000	0.0000	0.4616
	O4	8	4b	0.3333	0.6667	0.0117

T (K)	atom	Z	site	*x*	*y*	*z*
300	Lu1	71	2a	0.0000	0.0000	0.2697
	Lu2	71	4b	0.3333	0.6667	0.2287
	Mn	25	6c	0.3372	0.0000	0.0000
	O1	8	6c	0.3094	0.0000	0.1602
	O2	8	6c	0.6369	0.0000	0.3348
	O3	8	2a	0.0000	0.0000	0.4645
	O4	8	4b	0.3333	0.6667	0.0151