

Supplementary information

Distorted octahedron-dependent red-emitting $\text{Li}_2\text{K}_4\text{TiOGe}_4\text{O}_{12}:\text{Mn}^{4+}$ phosphor for White LEDs

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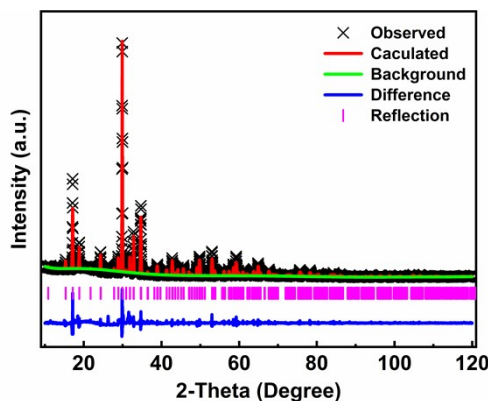


Fig. S1 XRD Rietveld refinement patterns of LKTGO.

Table S1. Rietveld fitting results of LKTGO and LKTGO:0.003Mn⁴⁺.

formula	LKTGO	LKTGO:0.003Mn ⁴⁺
crystal system	tetragonal	tetragonal
space group	<i>P4nc</i>	<i>P4nc</i>
<i>a</i> (Å)	11.5970(5)	11.62134(7)
<i>b</i> (Å)	11.5970(5)	11.62134(7)
<i>c</i> (Å)	5.1738(3)	5.184171(2)
$\alpha = \beta = \gamma$ (deg)	90	90
<i>Z</i>	2	2
<i>V</i> (Å ³)	695.82(8)	696.83(3)
<i>R_p</i>	0.0878	0.0708
<i>R_{wp}</i>	0.0998	0.0582
χ^2	14.04	6.888

Table S2. Atomic positions of LKTGO.

atom	x	y	z	occupancy	U_{iso}
Li	1	0.5	0.2729	1.000	0.0400
K	0.7662	0.9217	-0.0899	1.000	0.0160
Ti	1	1	0.4464	1.000	0.0043
Ge	0.7803	0.6084	-0.0603	1.000	0.0177
O1	0.8798	0.4827	-0.0984	1.000	0.0165
O2	0.6271	0.5904	0.0160	1.000	0.0837
O3	0.7670	0.6740	-0.3600	1.000	0.0583
O4	1	1	0.1132	1.000	0.0278

Table S3. Atomic positions of LKTGO:0.003Mn⁴⁺.

atom	x	y	z	occupancy	U_{iso}
Li	0.0000	0.5000	0.2511	1.0000	0.07778
K	0.7665	0.9225	-0.0710	1.0000	0.01812
Ti	1.0000	1.0000	0.3749	0.9948	0.00740
Ge	0.7816	0.6087	-0.0956	1.0000	0.01534
O1	0.8908	0.4810	-0.0500	1.0000	0.00681
O2	0.6302	0.5917	0.0124	1.0000	0.13379
O3	0.7542	0.6720	-0.3825	1.0000	0.06131
O4	1.0000	1.0000	0.7194	1.0000	0.00851
Mn	1.0000	1.0000	0.3749	0.0052	0.00740

Table S4. The calculated β_1 values and spectroscopic parameters of Mn⁴⁺ ions in various hosts.

Host	D_q	B	C	β_1	E (2E_g)	Ref
CaZrO ₃	1850	754	3173	0.983	15054	1
Ba ₂ GdNbO ₆	1931	855	2859	0.992	14793	2
CaAl ₁₂ O ₁₉	2132	807	3088	0.999	15244	3
SrGe ₄ O ₉	2362	832	3024	1.004	15267	4
Ca ₂ LaNbO ₆	1934	838	2827	0.976	14598	5
Sr ₂ MgGe ₂ O ₇	2387	833	2989	0.975	15175	6
La(MgTi) _{1/2} O ₃	2053	700	2959	0.915	14124	7
Mg ₂ Al ₄ Si ₅ O ₁₈	2141	927	2560	0.996	14705	8
K ₂ Ge ₄ O ₉	2163	785	3146	0.996	15281	9
CaMg ₂ La ₂ W ₂ O ₁₂	2088	731	2912	0.924	14124	10
LiAl ₅ O ₈	2014	725	2900	0.920	13977	11
YAlO ₃	2100	720	3025	0.938	14450	12
Y ₂ Sn ₂ O ₇	2100	700	3515	1.016	15563	13
SrMgAl ₁₀ O ₁₇	2237	791	3084	0.989	15152	14
YAl ₃ (BO ₃) ₄	1890	755	3015	0.956	14620	15
Li ₂ K ₄ TiOGe ₄ O ₁₂	2137	813	3007	0.990	15038	This work

Table S5. CIE coordinates of LKTGO:0.003Mn⁴⁺ at different temperature ($T = 298\text{--}473$ K).

Temperature (K)	CIE coordinates (x, y)
298	(0.719, 0.281)
323	(0.716, 0.283)
348	(0.711, 0.288)
373	(0.700, 0.298)
398	(0.676, 0.320)
423	(0.625, 0.366)
448	(0.552, 0.433)
473	(0.496, 0.484)

Table S6. The parameters of the prepared LED at various driving currents.

Current (mA)	Luminous efficiency (lm/W)
20	0.67
40	0.65
60	0.61
80	0.61
100	0.55
120	0.52
140	0.50
160	0.47
180	0.46
200	0.44
220	0.43
240	0.42
260	0.41
280	0.40
300	0.40

Table S7. The parameters of the prepared WLED at various driving currents.

Current (mA)	Luminous efficiency (lm/W)	CRI
20	56.89	90.20
30	56.20	88.52
40	55.08	87.60
50	54.06	86.08
60	53.66	84.80
70	52.88	83.28
80	52.02	81.30
90	51.66	80.08
100	51.23	78.60
110	50.12	77.08
120	50.11	75.56

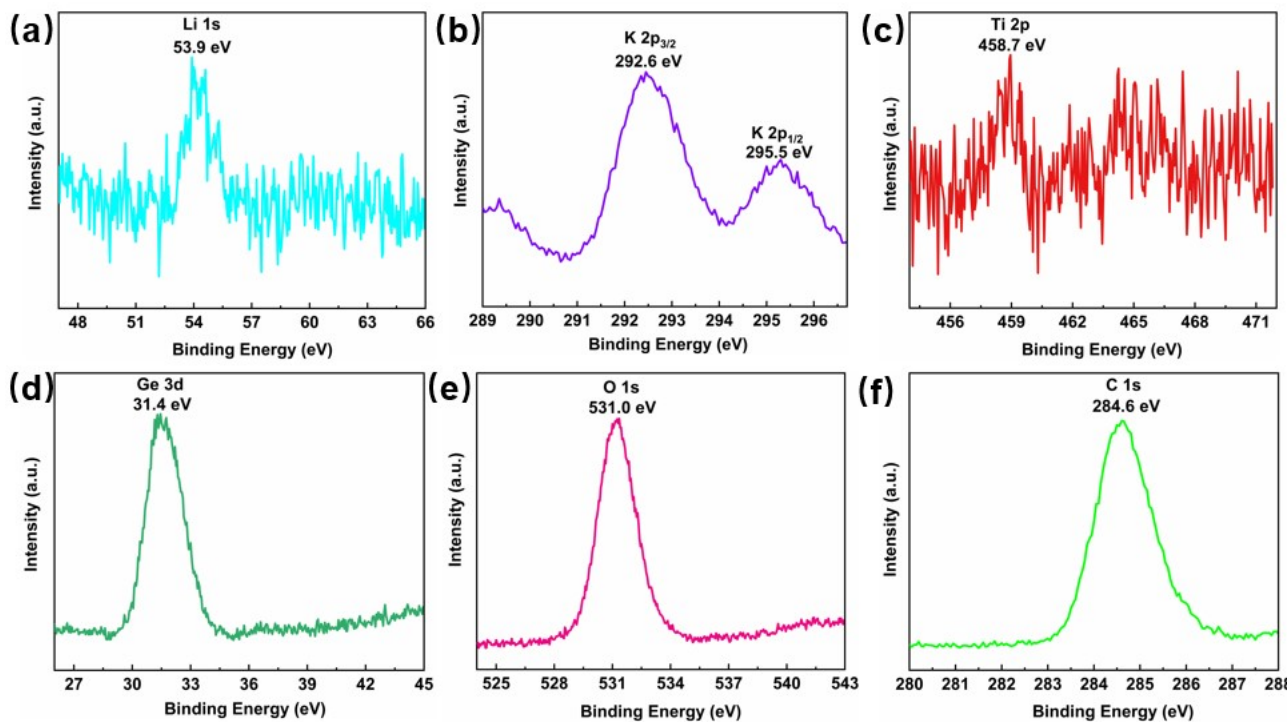


Fig. S2 XPS spectrogram of the LKTGO:0.003Mn⁴⁺ phosphors. (a) Li-1s, (b) K-2p, (c)Ti-2p, (d) Ge-3d, (e) O-1s and (f) C-1s.

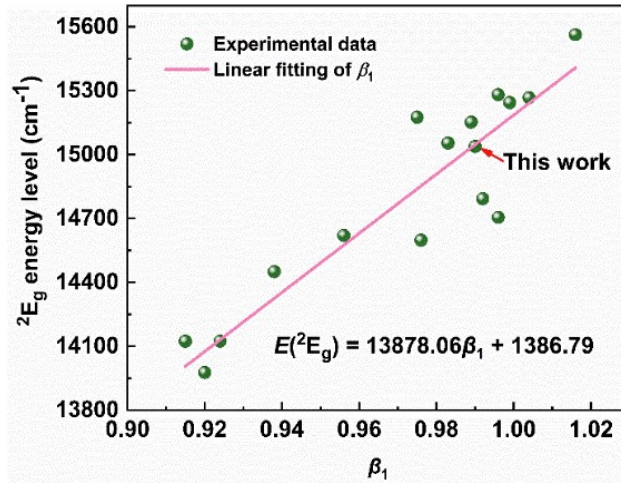


Fig. S3 Empirical relation between the nephelauxetic ratio β_1 and the energy position of the Mn^{4+} : 2E_g state in octahedral complexes.

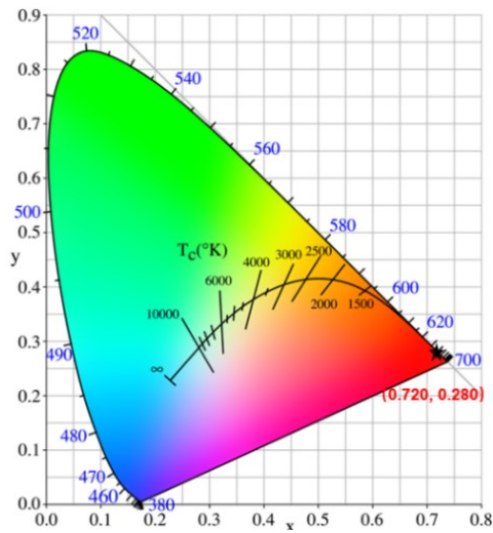


Fig. S4 CIE coordinates of LKTGO:0.003 Mn^{4+} phosphors at room temperature ($T = 273$).

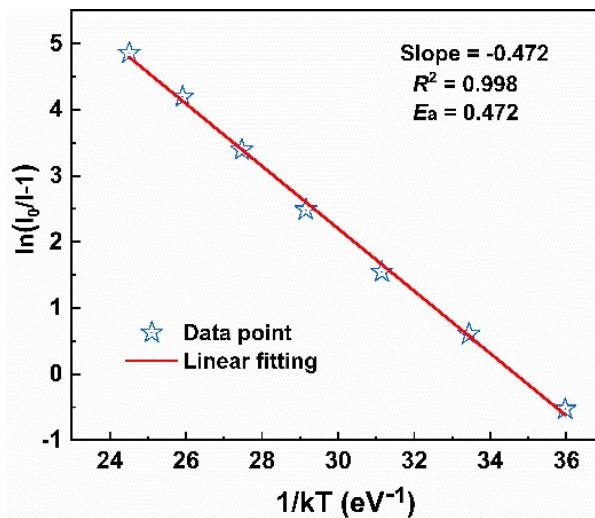


Fig. S5 The relationship of $\ln[(I_0/I_T)-1]$ with $1/T$ in LKTGO: $x\text{Mn}^{4+}$ phosphor.

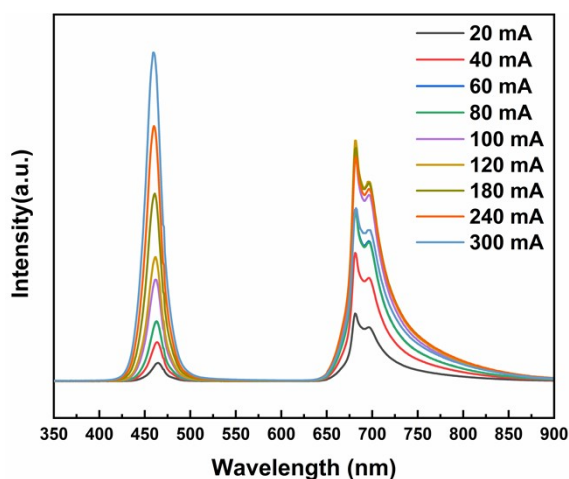


Fig. S6 PL spectra of the prepared LED at various driving currents.

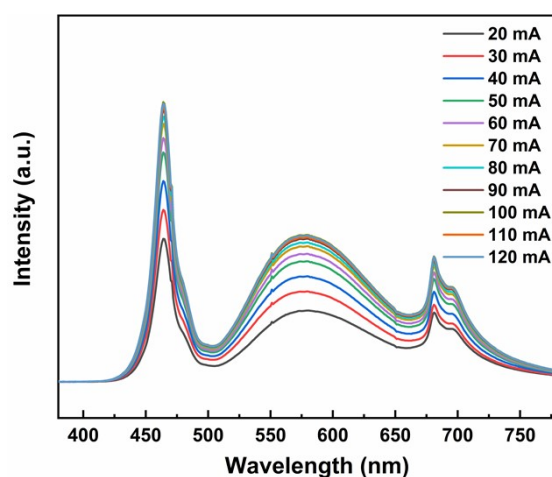


Fig. S7 PL spectra of the prepared WLED at various driving currents.

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