Electronic Supplementary Information

Construct a novel mechanoluminescent phosphor Li_2MgGeO_4:$x$$Mn^{2+}$ by defect control

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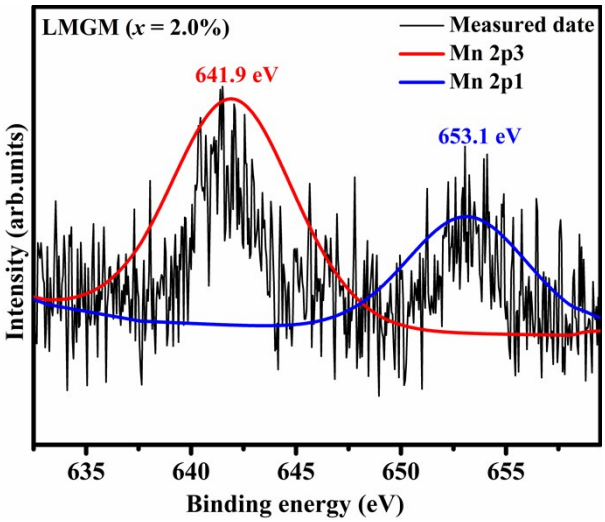

Fig. S1 High-resolution XPS spectra of Mn 2*p* for $Li_{2-x}MgGeO_4$:$x$$Mn^{2+}$ (x = 2.0%).

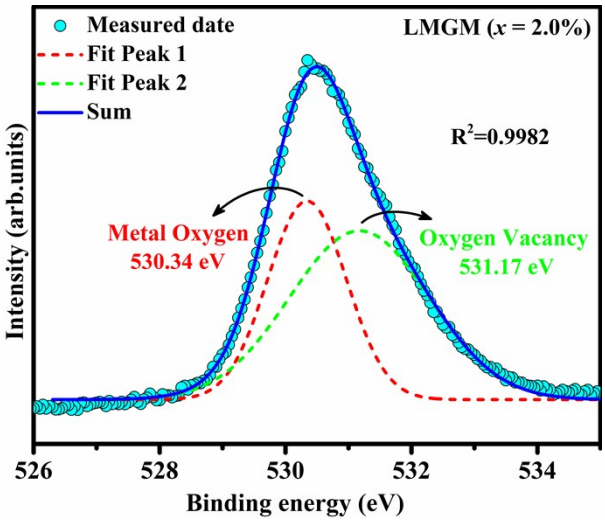

Fig. S2 High-resolution XPS spectra of O 1*s* for $Li_{2-x}MgGeO_4$:$x$$Mn^{2+}$ (x = 2.0%).

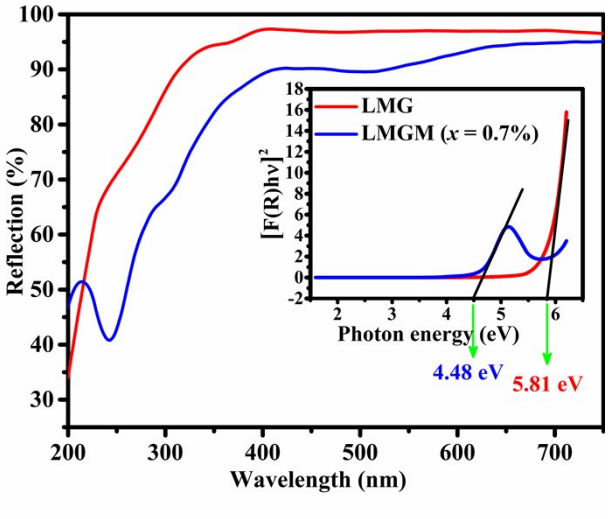

Fig. S3 The DR spectra of Li_2MgGeO_4 and $Li_{2-x}MgGeO_4$:xMn^{2+} (x = 0.7%).

The thermal stability of phosphors at high working temperature is a significant index to assess their application value.[1] As seen in Fig. S4a, the PL intensity decreases gradually with the increase in temperature owing the effect of thermal quenching, which reaches 66.8% at 100 °C and 44.9% at 150 °C of the initial intensity at 25 °C. Correspondingly, the activation energy can be calculated via the Arrhenius equation (Fig. S4b):

$$I_T = I_0/[1 + exp(-Ea/kT)] \quad (1)$$

where I_0 and I_T represent the PL intensities at room temperature and measuring temperature, respectively; E_a is the activation energy, k is the Boltzmann constant (8.617×10^{-5} eV·K^{-1}).[2] The value of 0.3096 eV reflects the acceptable thermal stability. Besides, the peak positions appear the tendency of blue-shift overall, which could be resulted from the lattice expansion at high temperature to lead to a decline in energy level splitting of Mn^{2+} ions.

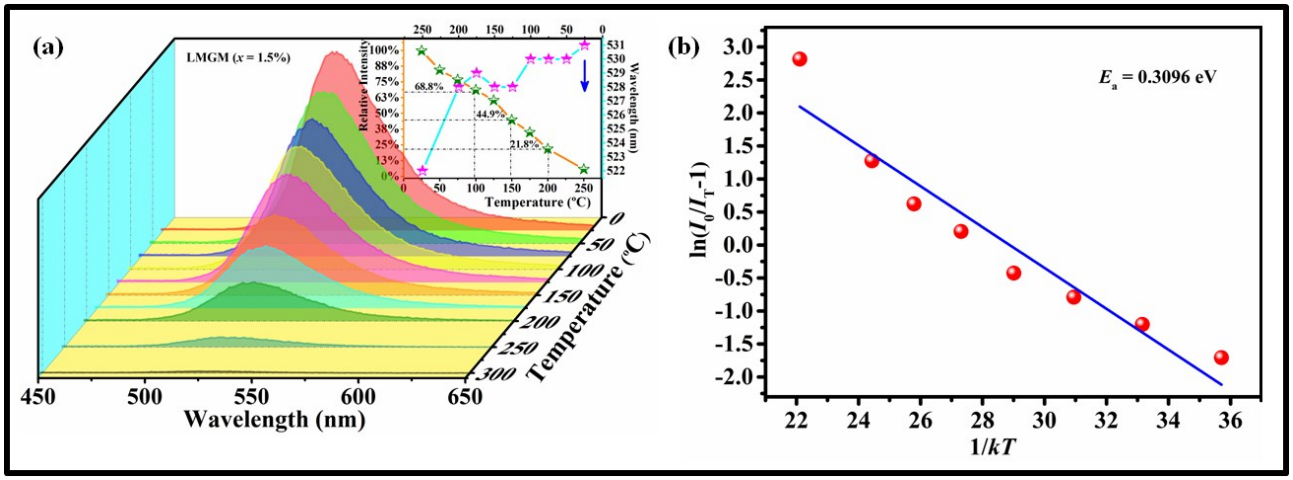

Fig. S4 (a) Temperature-dependent PL spectra under 256 nm excitation from 25 °C to 300 °C for $Li_{2-x}MgGeO_4$:xMn^{2+} (x = 1.5%); the inset shows the wavelength and intensity of peak versus temperature. (b) The ln(I_0/I_T−1) vs. 1/kT activation energy graph for thermal quenching of $Li_{2-x}MgGeO_4$:xMn^{2+} (x = 1.5%).

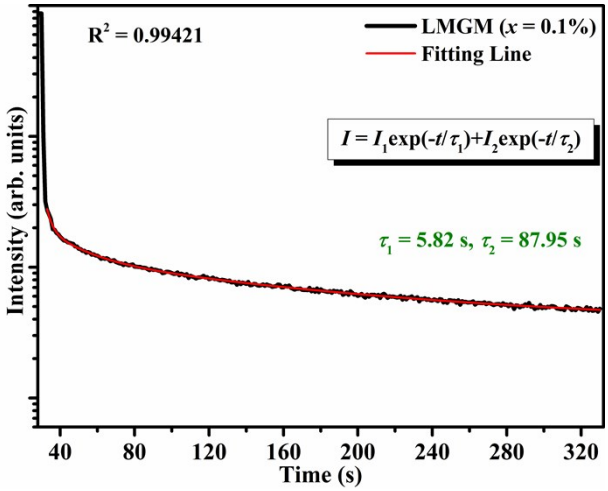

Fig. S5 The long persistent luminescence decay spectrum of $Li_{2-x}MgGeO_4$:xMn^{2+} (x = 0.1%).

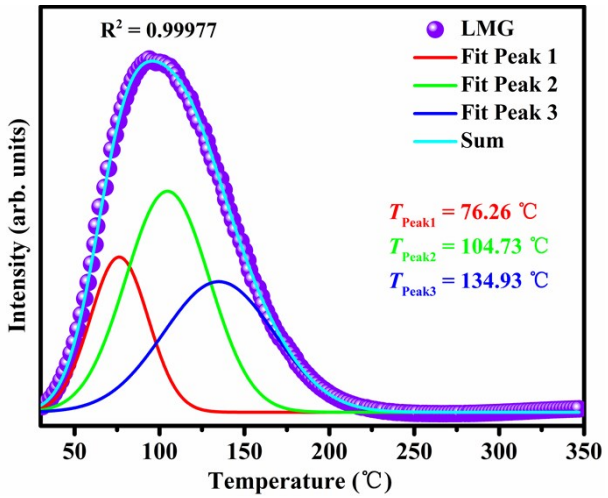

Fig. S6 ThL curve of Li_2MgGeO_4.

Table S1 Lattice parameters and agreement factors for Li_2MgGeO_4:xMn^{2+} (x = 1.5%) refined by Rietveld method, when Mn^{2+} ions occupy all kinds of the cationic sites.

Doped concentration	x = 0.015
Crystal system	orthorhombic
Space group	$Pmn2_1$
a (Å)	6.4042(2)
b (Å)	5.4686(2)
c (Å)	5.0063(16)
Volume (Å^3)	175.329(11)
Z	2
R_p (%)	13.35
R_{wp} (%)	18.08
S	1.35

Table S2 Lattice parameters and agreement factors for Li_2MgGeO_4:xMn^{2+} (x = 1.5%) refined by Rietveld method, when Mn^{2+} ions occupy the cationic sites of Li^+ and Mg^{2+}.

Doped concentration	$x = 0.015$
Crystal system	orthorhombic
Space group	$Pmn2_1$
a (Å)	6.3990(4)
b (Å)	5.4744(3)
c (Å)	5.0013(2)
Volume (Å^3)	175.198(15)
Z	2
R_p (%)	10.62
R_{wp} (%)	15.31
S	1.44

Table S3 Occupancy of Mn^{2+} occupying all the cationic sites for Li_2MgGeO_4:$x$$Mn^{2+}$ (x = 1.5%) refined by Rietveld method.

	Site	x	y	z	Occupancy
Li	4b	0.24948	0.16699	0.00234	0.9881(9)
Mn1	4b	0.24948	0.16699	0.00234	0.0119(9)
Mg	2a	0.000	0.3560(4)	0.4100(5)	1.00(7)
Mn2	2a	0.000	0.3560(4)	0.4100(5)	0.00(7)
Ge	2a	0.000	0.6719(9)	0.0280(4)	1.018(2)
Mn3	2a	0.000	0.6719(9)	0.0280(4)	-0.018(2)
O1	4b	0.2318	0.8238	0.8958	1.00
O2	2a	0.000	0.3150(8)	0.8950(7)	1.00
O3	2a	0.000	0.66978	0.35710	1.00

Table S4 Occupancy of Mn^{2+} occupying the cationic sites of Li^+ and Mg^{2+} for Li_2MgGeO_4:$x$$Mn^{2+}$ (x = 1.5%) refined by Rietveld method.

	Site	x	y	z	Occupancy
Li	4b	0.24948	0.16699	0.00234	0.98904(8)
Mn1	4b	0.24948	0.16699	0.00234	0.01096(8)
Mg	2a	0.000	0.3540(4)	0.4140(5)	1.00(6)
Mn2	2a	0.000	0.3540(4)	0.4100(5)	0.00(6)
Ge	2a	0.000	0.6689(9)	0.0090(2)	1.00
O1	4b	0.2020(2)	0.8470(4)	0.8890(2)	1.00
O2	2a	0.000	0.3170(7)	0.8920(7)	1.00
O3	2a	0.000	0.6950(6)	0.3500(2)	1.00

Table S5 Lattice parameters and agreement factors for $Li_{2-x}MgGeO_4$:$x$$Mn^{2+}$ (x = 0.015) refined by Rietveld method.

Doped concentration	$x = 0.015$
Crystal system	orthorhombic
Space group	$Pmn2_1$
a (Å)	6.39737(4)
b (Å)	5.47772(8)
c (Å)	4.99875(6)

Volume (Å^3)	175.17(10)
Z	2
R_p (%)	10.59
R_{wp} (%)	11.23
S	1.06

Table S6 Refined atomic positions for $Li_{2-x}MgGeO_4$:xMn^{2+} (x = 0.015).

	Np	x	y	z	Occupancy
Li	4	0.24948	0.16699	0.00234	0.98809(6)
Mn	4	0.24948	0.16699	0.00234	0.01191(6)
Mg	2	0.00000	0.33625(2)	0.50052(7)	1.0
Ge	2	0.00000	0.67423(4)	0.00679(2)	1.0
O1	4	0.21375(6)	0.82382(3)	0.89577(6)	1.0
O2	2	0.00000	0.36904(5)	0.89187(3)	1.0
O3	2	0.00000	0.66978(2)	0.35710(4)	1.0

References

1 X. Ji, J. Zhang, Y. Li, S. Liao, X. Zhang, Z. Yang, Z. Wang, Z. Qiu, W. Zhou, L. Yu and S. Lian, *Chem. Mater.*, 2018, **30**, 5137-5147.

2 M. Xin, Z. H. Huang, M. H. Fang, Y. G. Liu, C. Tang and X. W. Wu, *Inorg. Chem.*, 2014, **53**, 6060-6065.