Electronic Supplementary Information

Structure and Abnormal Photoluminescence of a Red-Emitting $LiMgBO_3$: Mn^{2+} phosphor

Liwei Wu[a], Yuxing Bai[a], Li Wu[a,*], Huan Yi[a], Xinzheng Zhang[a], Lixin Zhang[a], Yongfa Kong[a], Yi Zhang[b,*], Jingjun Xu[a]

[a]Key laboratory of Weak-Light Nonlinear Photonics, Ministry of Education, School of Physics, Nankai University, Tianjin 300071, China. Email: *lwu@nankai.edu.cn

[b]College of Electronic Information and Optical Engineering and Tianjin Key Laboratory of Photo-electronic Thin Film Devices and Technology, Nankai University, Tianjin 300071, China. Email: *yizhang@nankai.edu.cn

Table S1 Li(1)–O, Li(2)–O bonds valence of $LiMgBO_3$

	Li1	Li2
O1	0.2052	0.2808
O2	0.3258	0.2554
O3	0.3293	0.3171
	0.1464	0.0963
	0.0247	0.0373
$\sum s$	1.0314	0.9869

Table S2 Fractional Atomic Coordinates, Equivalent Isotropic Displacement Parameters ($Å^2$) and Occupancy for $LiMgBO_3$: $0.04Mn^{2+}$

	site	x	y	z	Ueq	occupancy
			$LiMgBO_3$: $0.04Mn^{2+}$			
Li1	8f	0.1968(11)	0.5104(7)	0.1509(3)	0.0299(6)	0.553(7)
Mn1	8f	0.1968(11)	0.5104(7)	0.1509(3)	0.0299(6)	0.022(7)
Li2	8f	0.1664(14)	0.4911(8)	0.1092(5)	0.0200(1)	0.407(4)
Mn2	8f	0.1664(14)	0.4911(8)	0.1092(5)	0.0200(1)	0.016(4)
Mg	8f	0.1560(2)	0.1668(1)	0.1244(1)	0.0236(3)	1.0000
B	8f	0.1613(6)	0.8271(3)	0.1287(2)	0.0465(5)	1.0000
O1	8f	0.4042(2)	0.3330(1)	0.0869(1)	0.0267(6)	1.0000
O2	8f	0.2893(2)	0.6930(1)	0.1635(1)	0.0446(9)	1.0000
O3	8f	0.3087(2)	0.9627(1)	0.1282(1)	0.0520(6)	1.0000

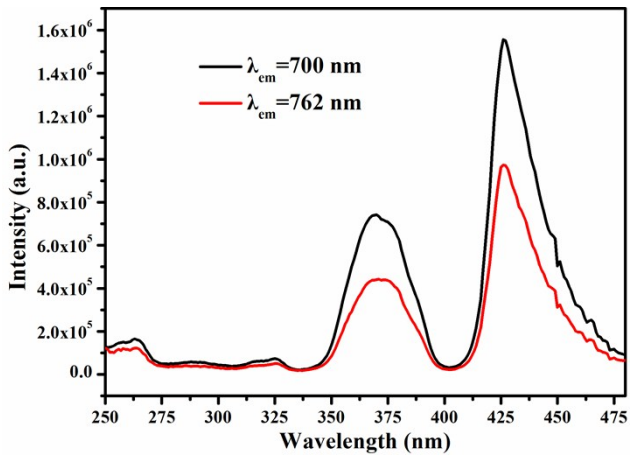

Figure S1 Excitation spectra of $LiMgBO_3$: $0.04Mn^{2+}$ monitored at 700 nm and 762 nm.

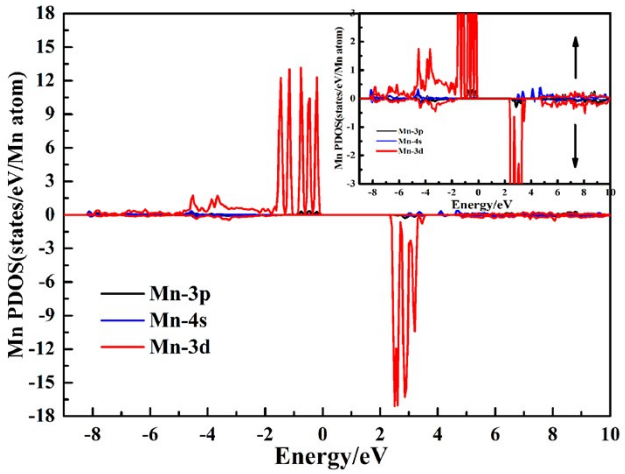

Figure S2 The orbital-decomposed DOS spectra of Mn ion in $LiMgBO_3$: 0.04Mn. The energy reference is set as the top of electron occupation. The upper and lower rows are corresponding to majority spin (spin-up) and minority spin (spin-down), respectively.

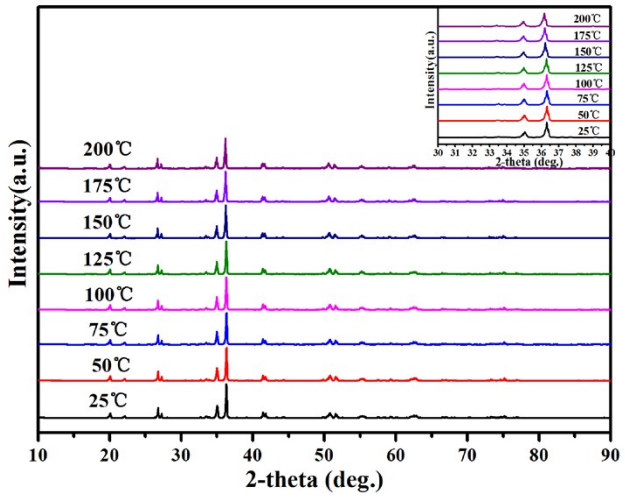

Figure S3 Temperature-dependent XRD patterns of $LiMgBO_3$: $0.04Mn^{2+}$.