Electronic supplementary information

Full visible light emission in Eu^{2+}, Mn^{2+} doped $Ca_9LiY_{0.667}(PO_4)_7$ phosphors based on multiple crystal lattice substitution and energy transfer for warm White LEDs with high Color-Rendering

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Table S1 Final refined atomic coordinates and occupancy for CLYPO:xEu^{2+} (x = 0 and 0.03) samples.

CLYPO					
atom	x	y	z	Occup.	B(Å^2)
Ca1	0.730256(2)	0.822118(5)	0.174525(2)	0.4720(2)	0.38(9)
Y1	0.730256(2)	0.822118(5)	0.174525(2)	0.5280(2)	0.38(9)
Ca2	0.63144(12)	0.822594(8)	-0.040468(3)	0.5316(7)	0.27(9)
Y2	0.63144(12)	0.822594(8)	-0.040468(3)	0.4684(7)	0.27(9)
Ca3	0.724181(9)	0.853069(1)	0.061623(6)	0.4970(3)	0.76(7)
Y3	0.724181(9)	0.853069(1)	0.061623(6)	0.5030(3)	0.76(7)
Ca4	0.000000(0)	0.000000(0)	-0.085100(0)	0.21239(6)	2.0(8)
Li1	0.000000(0)	0.000000(0)	-0.085100(0)	0.79761(6)	2.0(8)
Ca5	0.000000(0)	0.000000(0)	0.733600(2)	0.1321(5)	0.76(7)
Y3	0.000000(0)	0.000000(0)	0.733600(2)	0.8679(5)	0.76(7)
P1	0.000000(0)	0.000000(0)	-0.001872(6)	1.0	0.41(13)
P2	0.682370(9)	0.85480(8)	0.868049(3)	1.0	0.29(8)
P3	0.653730(4)	0.851891(6)	0.760547(2)	1.0	0.14(8)
O1	0.728957(5)	-0.103093(3)	-0.101869(1)	1.0	1.79(10)
O2	0.719960(4)	0.769974(6)	0.862686(10)	1.0	1.66(12)
O3	0.737938(3)	0.006864(6)	0.847058(2)	1.0	0.77(9)
O4	0.564690(2)	0.802872(5)	0.864536(7)	1.0	1.25(9)
O5	0.600829(4)	-0.082537(10)	0.780214(1)	1.0	0.44(8)
O6	0.562583(8)	0.681527(9)	0.776091(6)	1.0	1.32(10)
O7	0.098991(3)	0.927929(1)	0.779198(2)	1.0	0.27(7)
O8	0.625908(5)	0.825961(2)	0.726228(7)	1.0	0.84(8)
O9	0.016682(7)	0.879175(5)	-0.013030(2)	1.0	1.36(8)
O10	0.000000(0)	0.000000(0)	0.042563(1)	1.0	1.06(14)

CLYPO: Eu^{2+}					
atom	x	y	z	Occup.	B(Å^2)
Ca1	0.717272(2)	0.859331(5)	0.166463(6)	0.4985(3)	0.38(9)
Y1	0.717272(2)	0.859331(5)	0.166463(6)	0.4912(3)	0.38(9)
Eu1	0.717272(2)	0.859331(5)	0.166463(6)	0.0103(3)	0.38(9)
Ca2	0.624691(1)	0.824863(5)	-0.034543(8)	0.5041(4)	0.27(9)
Y2	0.624691(1)	0.824863(5)	-0.034543(8)	0.4805(4)	0.27(9)
Eu2	0.624691(1)	0.824863(5)	-0.034543(8)	0.0154(4)	0.27(9)
Ca3	0.733260(6)	0.838427(9)	0.082482(4)	0.4819(3)	0.76(7)
Y3	0.733260(6)	0.838427(9)	0.082482(4)	0.4706(3)	0.76(7)
Eu3	0.733260(6)	0.838427(9)	0.082482(4)	0.0475(3)	0.76(7)
Ca4	0.000000(0)	0.000000(0)	-0.085100(5)	0.27438(3)	2.0(8)
Li1	0.000000(0)	0.000000(0)	-0.085100(5)	0.72561(3)	2.0(8)
Ca5	0.000000(0)	0.000000(0)	0.733865(2)	0.1741(3)	0.76(7)
Y3	0.000000(0)	0.000000(0)	0.733865(2)	0.8127(3)	0.76(7)
Eu3	0.000000(0)	0.000000(0)	0.733865(2)	0.0132(3)	0.76(7)
P1	0.000000(0)	0.000000(0)	-0.006929(2)	1.0	0.41(13)
P2	0.688842(1)	0.859490(9)	0.867304(7)	1.0	0.29(8)
P3	0.651216(4)	0.841788(3)	0.767357(5)	1.0	0.14(8)
O1	0.725600(2)	-0.094400(4)	-0.091700(3)	1.0	1.79(10)
O2	0.767400(1)	0.783300(2)	0.854800(5)	1.0	1.66(12)
O3	0.729800(4)	0.008800(6)	0.848600(7)	1.0	0.77(9)
O4	0.522100(3)	0.760800(4)	0.862700(7)	1.0	1.25(9)
O5	0.598700(1)	-0.048800(3)	0.779400(5)	1.0	0.44(8)
O6	0.573800(3)	0.693000(4)	0.785000(6)	1.0	1.32(10)
O7	0.080300(7)	0.899000(3)	0.777100(2)	1.0	0.27(7)
O8	0.632000(4)	0.825800(2)	0.726800(5)	1.0	0.84(8)
O9	0.005700(5)	0.862400(3)	-0.011500(1)	1.0	1.36(8)
O10	0.000000(0)	0.000000(0)	0.042100(8)	1.0	1.06(14)

Table S2. Crystallographic parameters obtained from XRD Rietveld refinements for CLYPO:xEu^{2+} (x = 0 and 0.03)

	crystallographic parameter					reliability factors	
samples	a/b (Å)	c(Å)	V(Å)	α/β(deg)	γ(deg)	Rwp (%)	Rp (%)
x = 0	10.4078 (2)	37.2444(5)	3493.89	90	120	6.30	7.1
x = 0.03	10.4123(2)	37.2664(5)	3498.98	90	120	4.84	6.48
Crystal system	hexagonal						
Space group	R 3 c						

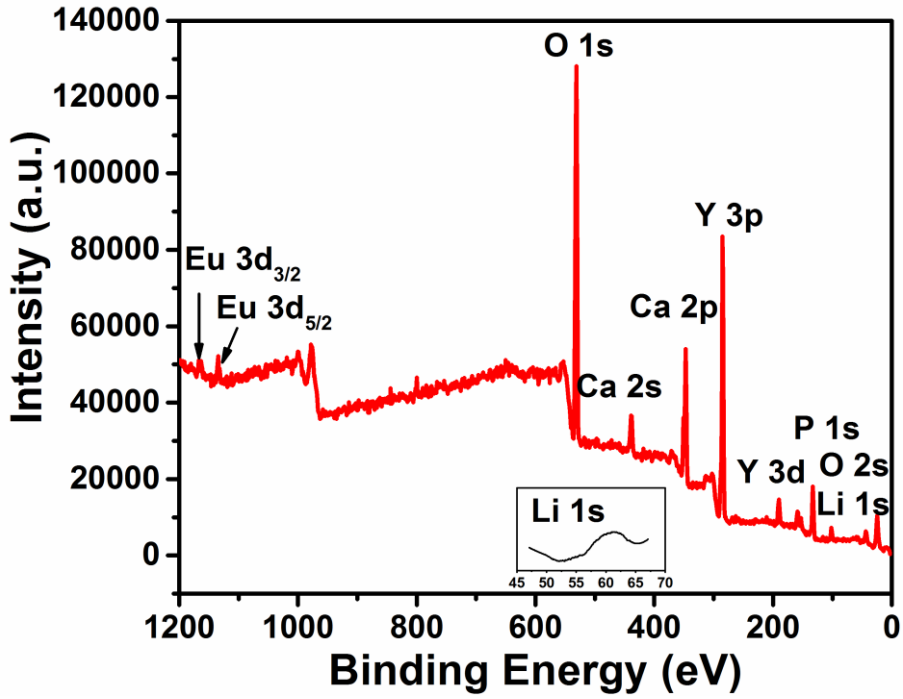

Fig. S1 XPS survey spectra of CLYPO: $0.03Eu^{2+}$ phosphor.

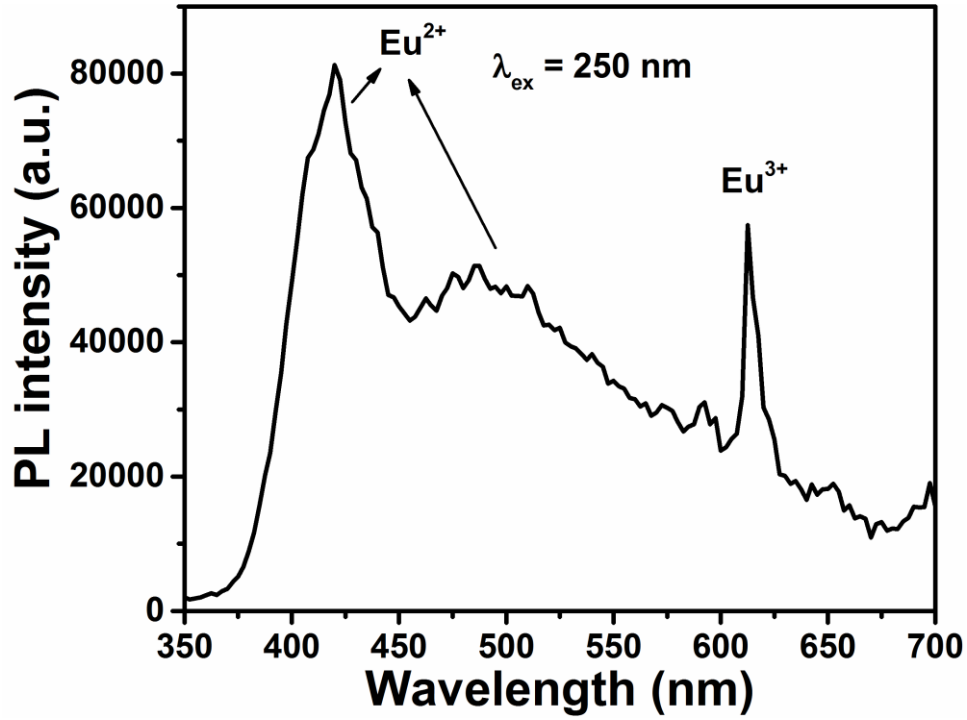

Fig. S2. The emission spectrum of CLYPO: $0.03Eu^{2+}$ sample.

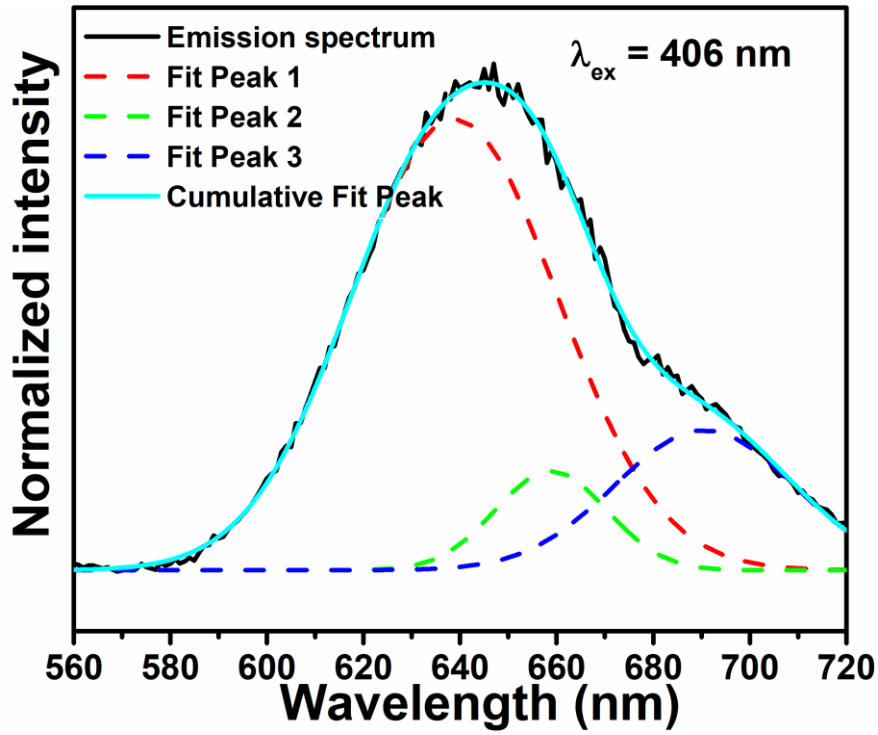

Fig. S3. The emission spectrum and Gaussian fitting spectra of CLYPO: $0.10Mn^{2+}$.

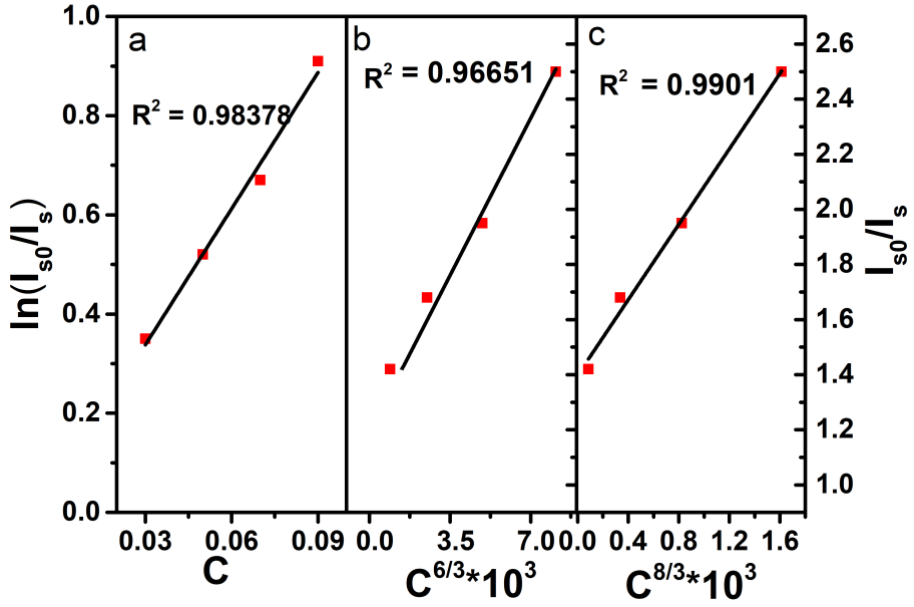

Fig. S4. Dependence of (a) $\ln(I_{S0}/I_S)$ of Eu^{2+} on C, and that of I_{S0}/I_S of Eu^{2+} on (b) $C^{6/3}$, (c) $C^{8/3}$.

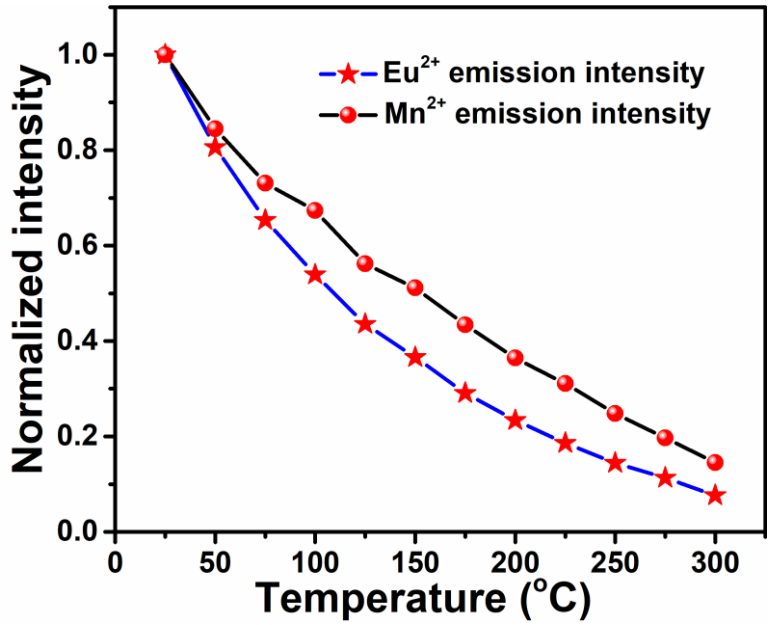

Fig. S5. Emission intensity for Eu^{2+} and Mn^{2+} in CLYPO: $0.03Eu^{2+}$, $0.03Mn^{2+}$ sample as a function of temperature.

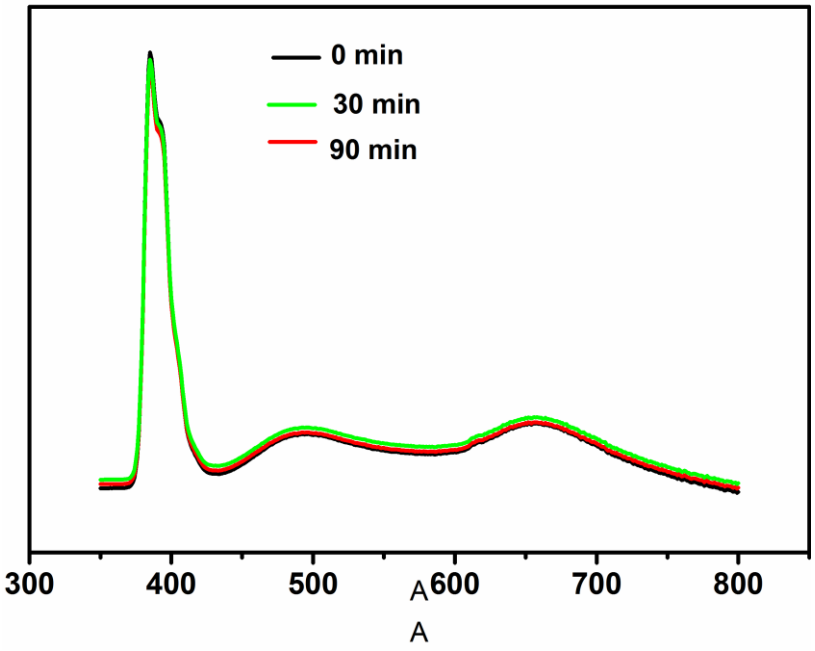

Fig. S6 Electroluminescent (EL) spectra of the as-fabricated and lighted WLEDs based on white emitting CLYPO:0.03Eu^{2+}, 0.05Mn^{2+} samples with different lighted time.