Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Site Occupancy and Luminescence Properties of $Ca_3Ln(AlO)_3(BO_3)_4:Ce^{3+},Tb^{3+},Mn^{2+}$ (Ln = Y, Gd) Phosphors for White-LEDs

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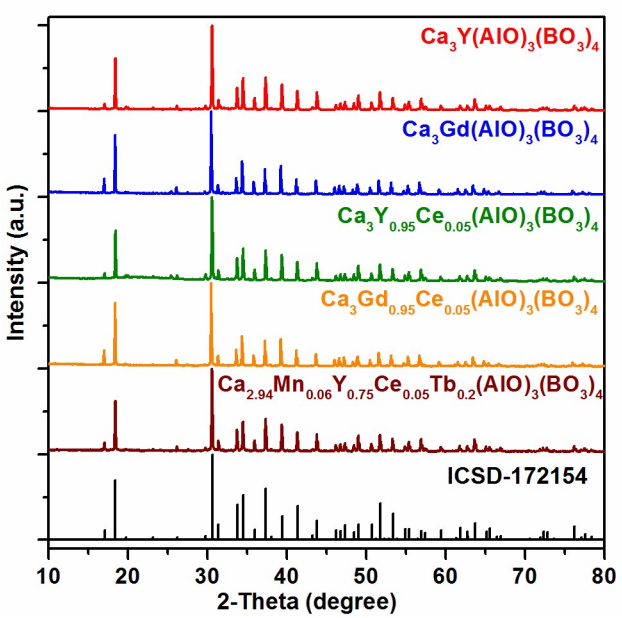

Figure S1. XRD patterns of $Ca_3Ln(AlO)_3(BO_3)_4$:Ce^{3+},Tb^{3+},Mn^{2+} phosphors.

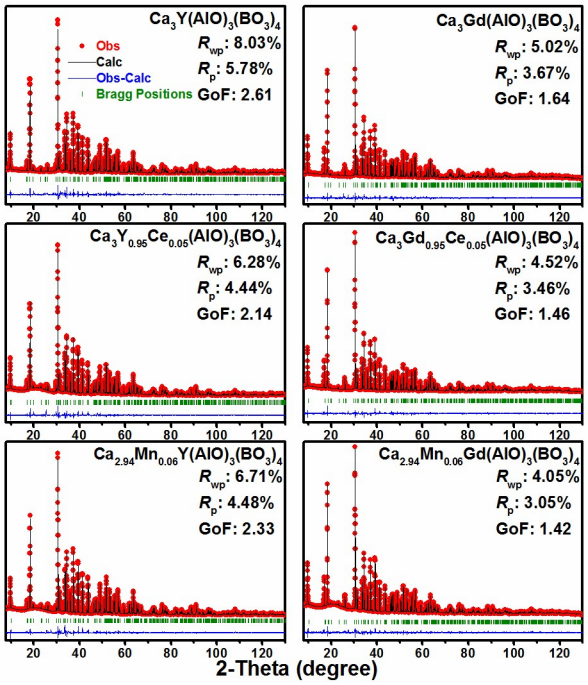

Figure S2. Rietveld refinement results of $Ca_3Ln(AlO)_3(BO_3)_4$:Ce^{3+},Mn^{2+}.

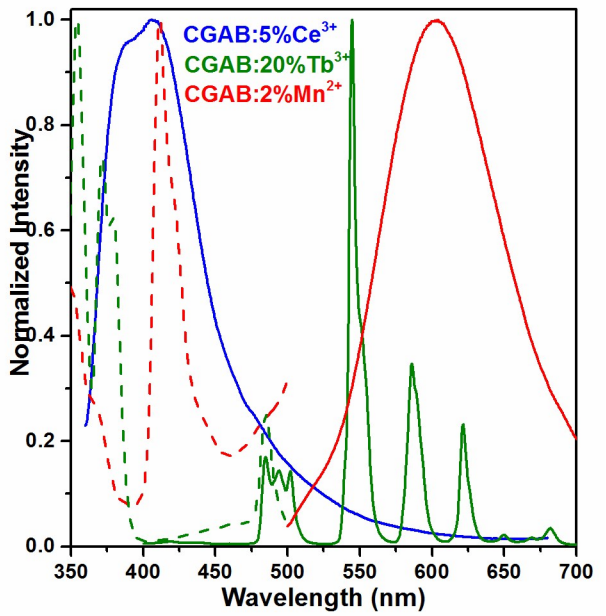

Figure S3. PL spectra (solid lines) of CGAB:5%Ce^{3+} (λ_{Ex} = 350 nm), CGAB:20%Tb^{3+} (λ_{Ex} = 354 nm) and CGAB:2%Mn^{2+} (λ_{Ex} = 411 nm) and corresponding PLE spectra (dashed lines) monitored at 545 nm (CGAB:20%Tb^{3+}) and 606 nm (CGAB:2%Mn^{2+}).

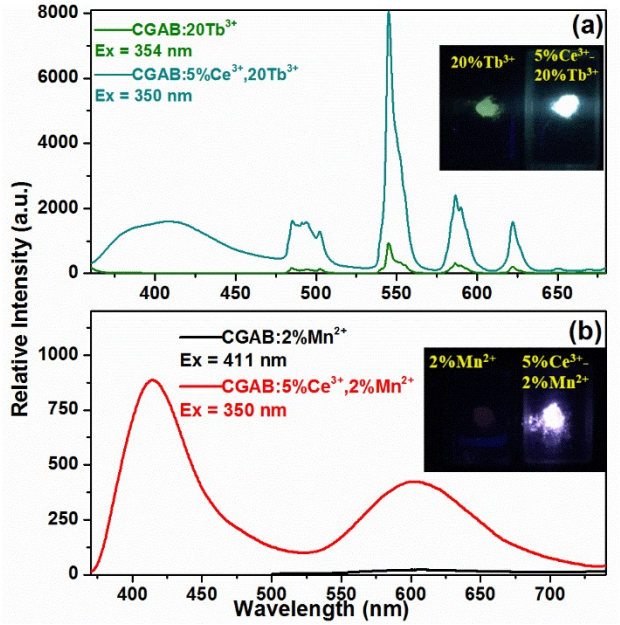

Figure S4. PL emission and corresponding photos of CGAB:20%Tb^{3+}, CGAB:5%Ce^{3+},Tb^{3+} (a) and CGAB:2%Mn^{2+}, CGAB:5%Ce^{3+},2%Mn^{2+} (b).

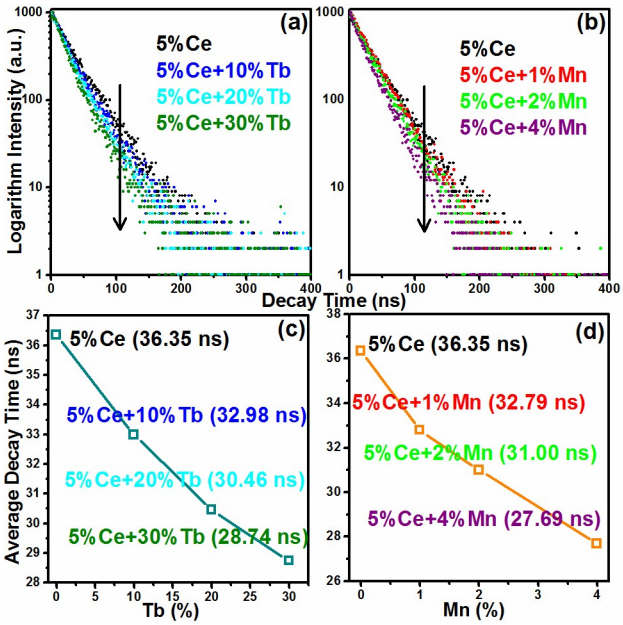

Figure S5. Luminescence decay curves of Ce^{3+} emission in CYAB:5%Ce,0%~30%Tb (a) and CYAB:5%Ce,0%~4%Mn (b), and the corresponding average decay times (c) and (d).

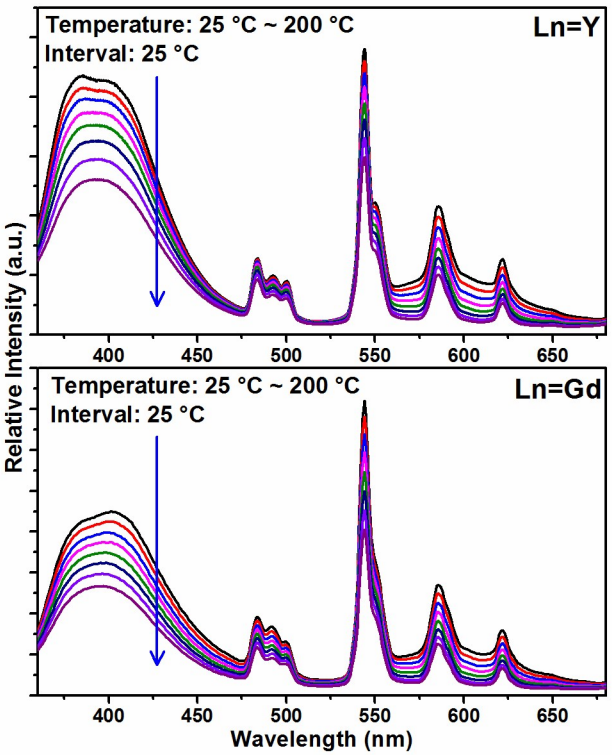

Figure S6. Temperature dependence of the PL spectra of CLnAB:5%Ce^{3+},20%Tb^{3+},2%Mn^{2+}. (λ_{Ex} = 350 nm)

Table S1. Parameters from Rietveld refinement of the $Ca_3Y(AlO)_3(BO_3)_4$.

Space Group	$P6_3/m$ (NO.176)				
a, c (Å)	10.38941(6), 5.69310(6)				
Atom	x	y	z	Fraction	U_{iso} (Å^2)[a]
Ca1/Y1	0.3333	0.6667	0.25	0.234(5)/0.766(5)	0.41(5)
Ca2/Y2	0.12901(22)	0.84140(21)	0.25	0.921(2)/0.078(2)	0.81(5)
Al	0	0.5	0	1	0.57(6)
B1	0.2171(13)	0.7656(14)	0.75	1	0.11(2)
B2	0	0	0.094(4)	0.5	0.11(2)
O1	0.0897(6)	0.4728(5)	0.25	1	0.84(16)
O2	0.3434(7)	0.9208(6)	0.75	1	1.79(17)
O3	0.3063(4)	0.4764(4)	0.5322(6)	1	1.36(11)
O4	0.0663(13)	0.9120(13)	0.5997(10)	0.5	0.33(18)

[a]The U_{iso} values have been multiplied by 100.

Table S2. Parameters from Rietveld refinement of the $Ca_3Gd(AlO)_3(BO_3)_4$.

Space Group	$P6_3/m$ (NO.176)				
a, *c* (Å)	10.4431(10), 5.7126(6)				
Atom	*x*	*y*	*z*	Fraction	U_{iso} (Å^2)[a]
Ca1/Gd1	0.3333	0.6667	0.25	0.277(5)/0.723(5)	0.32(6)
Ca2/Gd2	0.12948(32)	0.84283(32)	0.25	0.907(2)/0.093(2)	2.17(10)
Al	0	0.5	0	1	0.93(9)
B1	0.2137(18)	0.7545(21)	0.75	1	0.74(33)
B2	0	0	0.098(5)	0.5	0.74(33)
O1	0.0891(9)	0.4745(8)	0.25	1	1.91(25)
O2	0.3514(11)	0.9222(10)	0.75	1	4.31(30)
O3	0.3003(6)	0.4721(5)	0.5376(7)	1	1.42(17)
O4	0.0703(23)	0.9178(23)	0.5947(15)	0.5	1.08(26)

[a]The U_{iso} values have been multiplied by 100.

Table S3. Parameters from Rietveld refinement of the $Ca_3Y_{0.95}Ce_{0.05}(AlO)_3(BO_3)_4$.

Space Group	$P6_3/m$ (NO.176)				
a, c (Å)	10.3985(9), 5.6975(5)				
Atom	x	y	z	Fraction	U_{iso} (Å^2)[a]
Ca1/Y1/				0.281(3)/0.719/	
Ce1	0.3333	0.6667	0.25	0.000(3)	0.36(8)
Ca2/Y2/				0.906(1)/0.077/	
Ce2	0.12940(25)	0.84289(24)	0.25	0.017(1)	1.70(9)
Al	0	0.5	0	1	1.02(10)
B1	0.2219(14)	0.7634(16)	0.75	1	0.19(15)
B2	0	0	0.102(4)	0.5	0.19(15)
O1	0.0918(6)	0.4751(6)	0.25	1	0.83(19)
O2	0.3443(7)	0.9171(6)	0.75	1	1.36(18)
O3	0.3005(4)	0.4746(4)	0.5387(6)	1	0.35(13)
O4	0.0644(13)	0.9119(12)	0.6012(11)	0.5	0.19(15)

[a]The U_{iso} values have been multiplied by 100.

Table S4. Parameters from Rietveld refinement of the $Ca_3Gd_{0.95}Ce_{0.05}(AlO)_3(BO_3)_4$.

Space Group	$P6_3/m$ (NO.176)				
a, *c* (Å)	10.4435(8), 5.7103(4)				
Atom	*x*	*y*	*z*	Fraction	U_{iso} (Å^2)[a]
Ca1/Gd1/				0.241(1)/0.757/	
Ce1	0.3333	0.6667	0.25	0.002(1)	0.10(7)
Ca2/Gd2/				0.919(3)/0.0645/	
Ce2	0.12947(25)	0.84302(25)	0.25	0.016 (1)	1.14(9)
Al	0	0.5	0	1	0.75(10)
B1	0.2253(19)	0.7653(20)	0.75	1	0.12(11)
B2	0	0	0.099(4)	0.5	0.12(11)
O1	0.0908(7)	0.4718(6)	0.25	1	0.75(10)
O2	0.3426(8)	0.9175(7)	0.75	1	0.12(11)
O3	0.3025(5)	0.4741(4)	0.5382(6)	1	0.12(11)
O4	0.0642(16)	0.9149(16)	0.6028(12)	0.5	0.12(11)

[a]The U_{iso} values have been multiplied by 100.

Table S5. Parameters from Rietveld refinement of the $Ca_{2.94}Mn_{0.06}Y(AlO)_3(BO_3)_4$.

Space Group	$P6_3/m$ (NO.176)				
a, *c* (Å)	10.3966(8), 5.6972(4)				
Atom	*x*	*y*	*z*	Fraction	U_{iso} (Å^2)[a]
Ca1/Y1/				0.236/0.702(7)/	
Mn1	0.3333	0.6667	0.25	0.059(7)	0.15(7)
Ca2/Y2/				0.901/0.999(2)/	
Mn2	0.12859(22)	0.84195(22)	0.25	0.000(2)	1.36(8)
Al	0	0.5	0	1	0.83(8)
B1	0.2261(14)	0.7693(15)	0.75	1	0.40(20)
B2	0	0	0.094(4)	0.5	0.40(20)
O1	0.0900(6)	0.4696(5)	0.25	1	0.83(8)
O2	0.3377(6)	0.9170(6)	0.75	1	0.23(15)
O3	0.3030(4)	0.4749(4)	0.5379(5)	1	0.35(12)
O4	0.0631(12)	0.9134(11)	0.6031(10)	0.5	0.20(18)

[a]The U_{iso} values have been multiplied by 100.

Table S6. Parameters from Rietveld refinement of the $Ca_{2.94}Mn_{0.06}Gd(AlO)_3(BO_3)_4$.

Space Group	P63/*m* (NO.176)				
a, *c* (Å)	10.44335(20), 5.71168(12)				
Atom	*x*	*y*	*z*	Fraction	U_{iso} (Å^2)[a]
Ca1/Gd1/				0.165/0.783(5)/	
Mn1	0.3333	0.6667	0.25	0.052(5)	0.56(5)
Ca2/Gd2/				0.925/0.073(2)/	
Mn2	0.12890(31)	0.84271(31)	0.25	0.003(2)	1.72(9)
Al	0	0.5	0	1	1.26(9)
B1	0.2247(23)	0.7687(25)	0.75	1	1.01(29)
B2	0	0	0.095(5)	0.5	1.01(29)
O1	0.0881(8)	0.4696(7)	0.25	1	0.45(21)
O2	0.3403(9)	0.9187(8)	0.75	1	0.96(21)
O3	0.3028(5)	0.4737(4)	0.5390(7)	1	0.31(14)
O4	0.0666(22)	0.9175(22)	0.6015(14)	0.5	0.73(25)

[a]The U_{iso} values have been multiplied by 100.

Table S7. Interatomic bond distance of M1-O and M2-O in CGAB:5%Ce^{3+}, CYAB:2%Mn, and CGAB:2%Mn.

Bond	Length (Å)		
	CGAB:5%Ce	CYAB:2%Mn	CGAB:2%Mn
M1-O1	2.324 (×3)	2.327 (×3)	2.350 (×6)
M1-O3	2.492 (×6)	2.477 (×6)	2.499 (×3)
M2-O1	2.358 (×1)	2.338 (×1)	2.361 (×1)
M2-O2	2.558 (×1)	2.508 (×1)	2.526 (×1)
M2-O3	2.425 (×2)	2.417 (×2)	2.428 (×2)
M2-O4	2.366 (×1)	2.352 (×1)	2.361 (×1)
M2-O4	2.368 (×1)	2.360 (×1)	2.395 (×1)
M2-O4	2.432 (×1)	2.431 (×1)	2.410 (×1)