Electronic Supplementary Material (ESI) for CrystEngComm.

Improvement the thermal stability of bluish-cyan emitting phosphor $Y_2MgAl_4SiO_{12}:Eu^{2+}$ using substitution cations (Zn, Ca, Sr) for white LEDs

Huifang Yang[1], Panlai Li[1]*, Zejun Ye[1], Xiaoxue Huo[1], Yu Wang[1], Qian Wu[1], Dawei Wang[2], Jinxin Zhao[2], Fenghe Wang[1]*, Zhijun Wang[1]*

[1]*Hebei Key Laboratory of Optic-electronic Information and Materials, College of Physics Science & Technology, Hebei University, Baoding 071002, China*

[2]*Hebei Key Laboratory of Semiconductor Lighting and Display Critical Materials, Baoding, 071000, China*

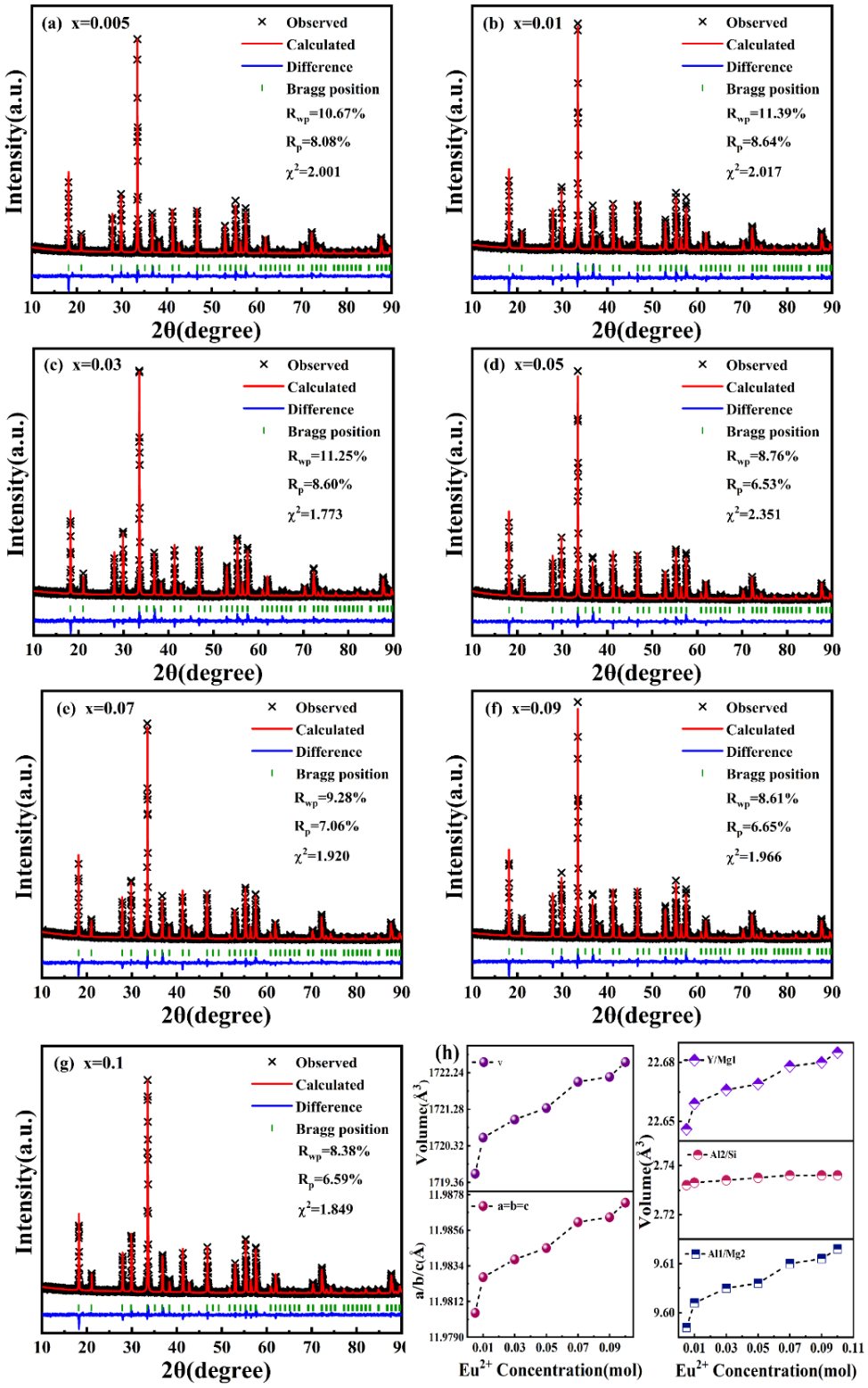

Fig. S1 (a-g) Refinement diagram of YMAS: xEu^{2+}(x=0.005-0.1); (h) Cell volume change trend diagram.

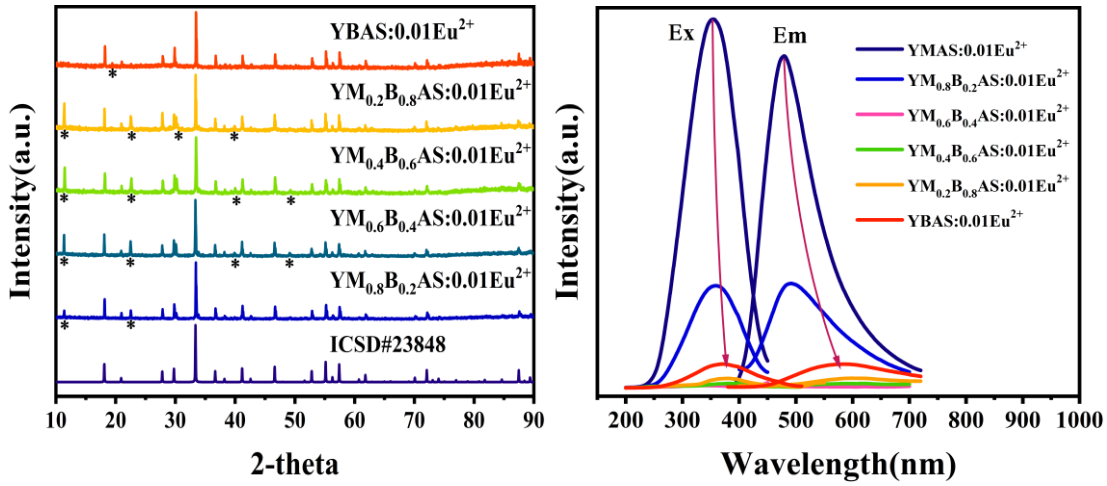

Fig. S2 XRD patterns of $Y_2(Mg, Ba)Al_4SiO_{12}:0.01Eu^{2+}$; Excitation and emission spectra of $Y_2(Mg, Ba)Al_4SiO_{12}:0.01Eu^{2+}$ phosphor.

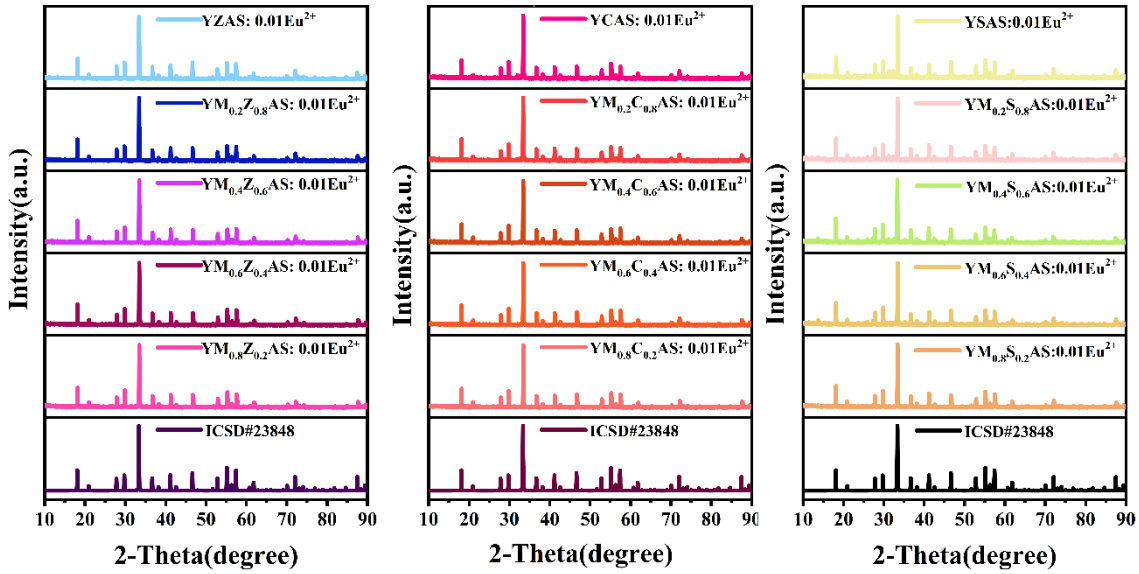

Fig. S3 XRD patterns of $Y_2Mg_{1-y}M_yAl_4SiO_{12}$: $0.01Eu^{2+}$ (M = Zn, Ca, Sr, y = 0, 0.2, 0.4, 0.6, 0.8, 1).

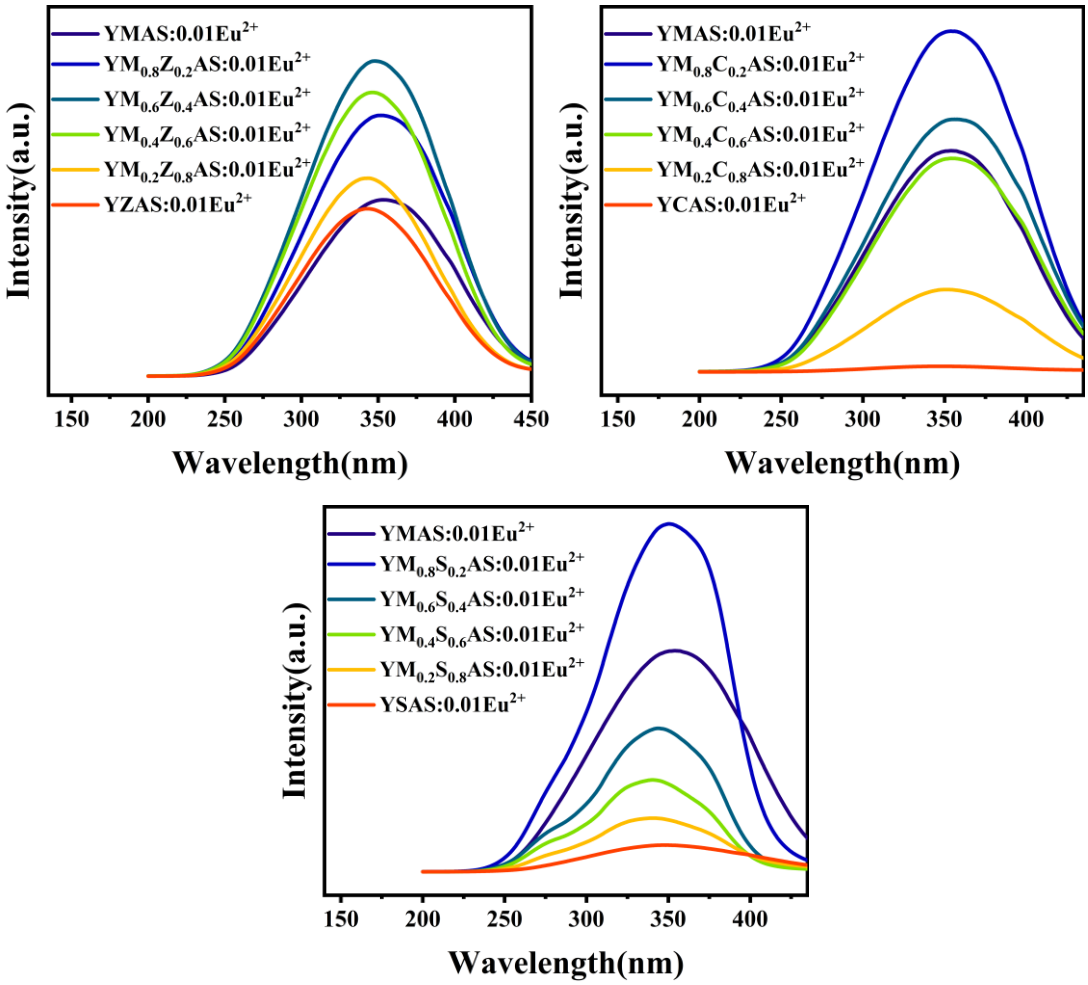

Fig. S4 Excitation spectra of $Y_2Mg_{1-y}M_yAl_4SiO_{12}$:0.01$Eu^{2+}$ (M=Zn, Ca, Sr) (y=0, 0.2, 0.4, 0.6, 0.8,1) monitoring emission at 470 nm.

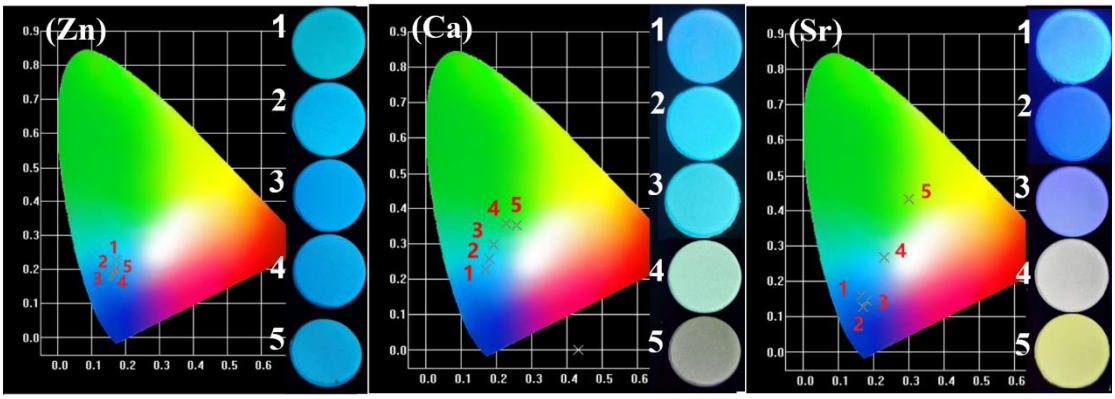

Fig. S5 CIE coordinates of $Y_2Mg_{1-y}M_yAl_4SiO_{12}$: $0.01Eu^{2+}$ (M = Zn, Ca, Sr, y = 0.2, 0.4, 0.6, 0.8, 1) and photograph under UV light of 365nm.

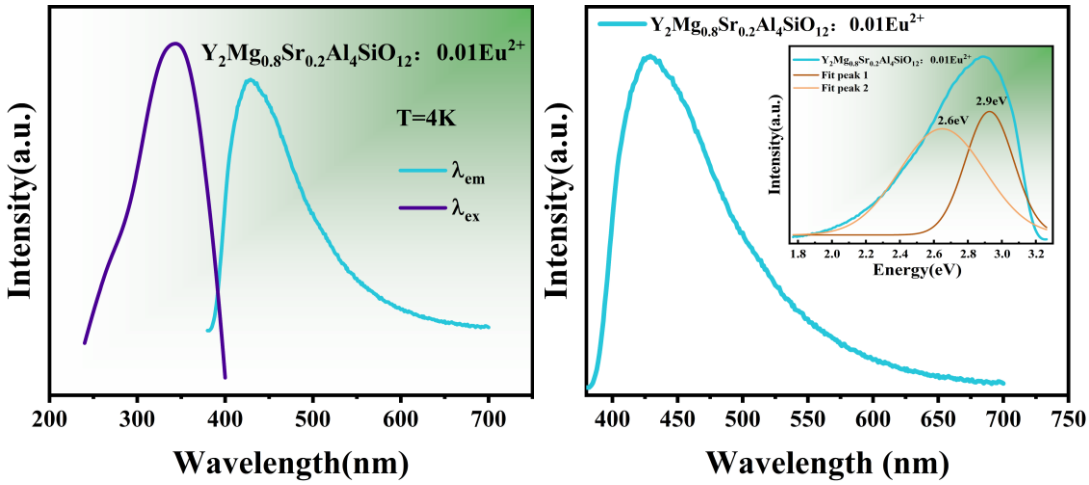

Fig. S6 Excitation and emission spectra of $Y_2Mg_{0.8}Sr_{0.2}Al_4SiO_{12}$:0.01$Eu^{2+}$ phosphor at low temperature 4K and Gaussian fitting result at low temperature 4K.

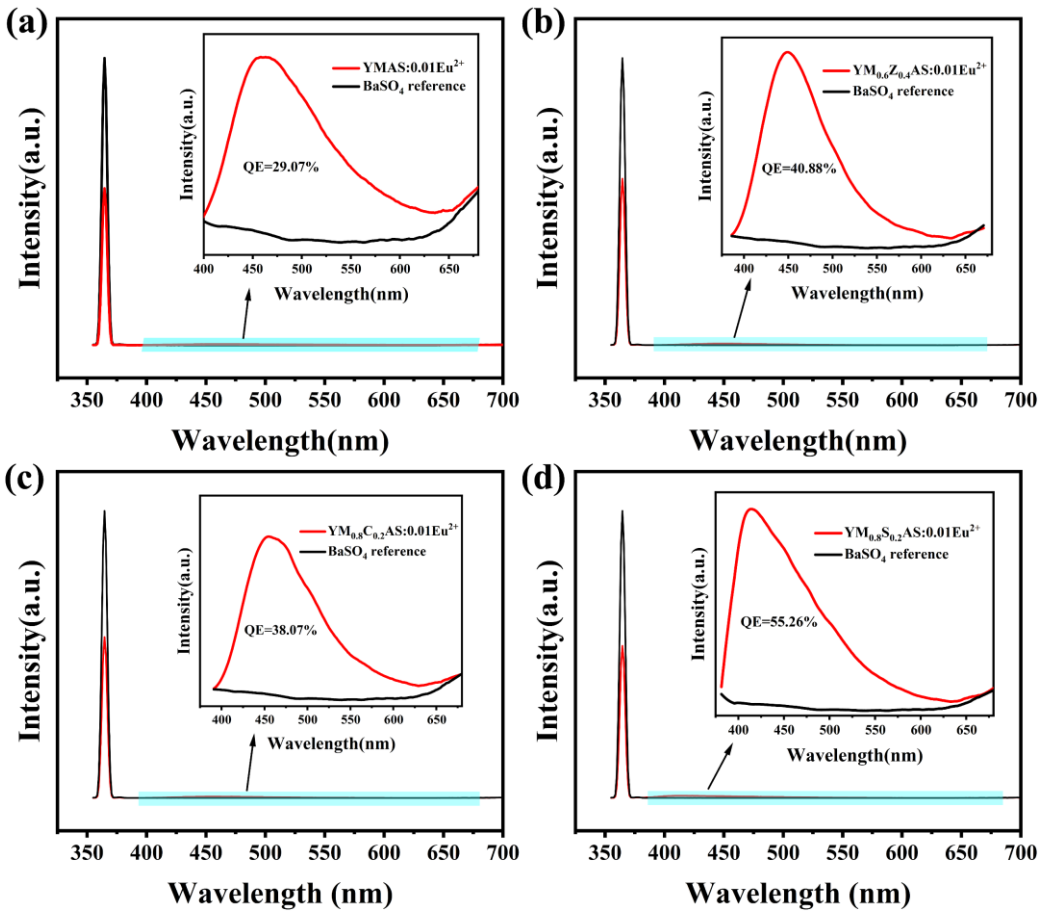

Fig.S7 Quantum efficiency using the HORIBA FLuorolog-3 fluorescence spectrometer and Quanta–φ integrating sphere.

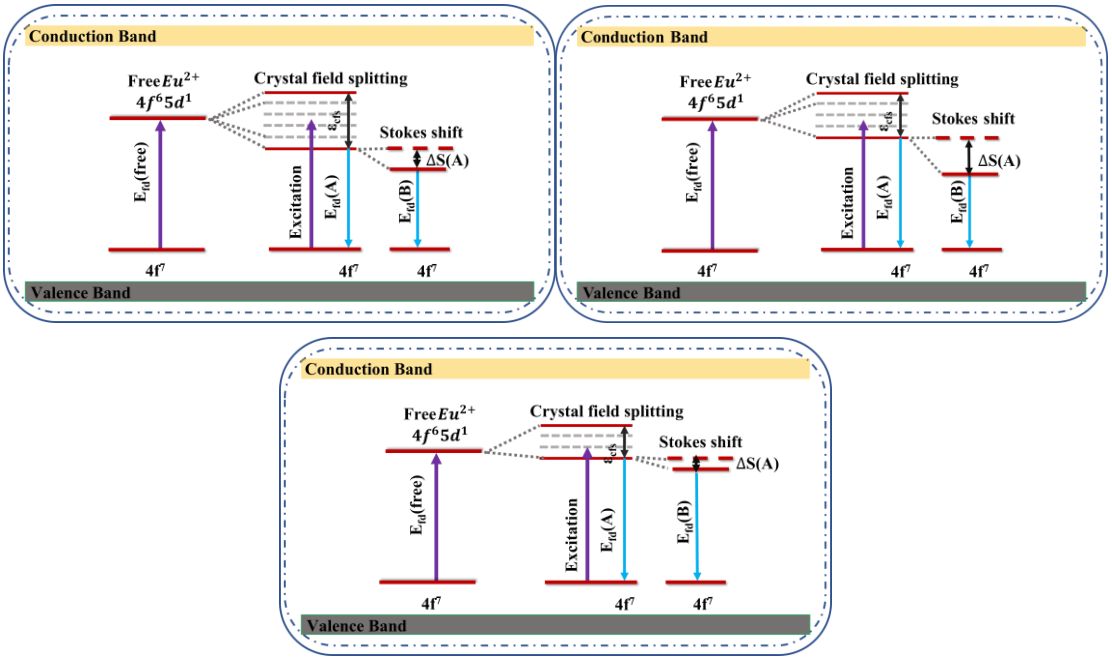

Fig. S8 Eu^{2+} electron transition level structure diagram in $Y_2Mg_{0.6}Zn_{0.4}Al_4SiO_{12}$:0.01$Eu^{2+}$, $Y_2Mg_{0.8}Ca_{0.2}Al_4SiO_{12}$:0.01$Eu^{2+}$ and $Y_2Mg_{0.8}Sr_{0.2}Al_4SiO_{12}$:0.01 Eu^{2+}.

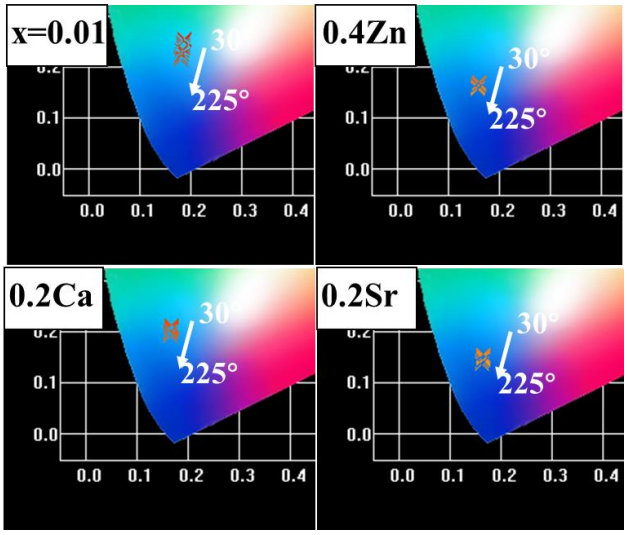

Fig. S9 Chromaticity coordinates of the YMAS:0.01Eu^{2+}, $Y_2Mg_{0.6}Zn_{0.4}Al_4SiO_{12}$:0.01$Eu^{2+}$, $Y_2Mg_{0.8}Ca_{0.2}Al_4SiO_{12}$:0.01$Eu^{2+}$ and $Y_2Mg_{0.8}Sr_{0.2}Al_4SiO_{12}$:0.01 Eu^{2+} in temperature range of 30°C to 225 °C.

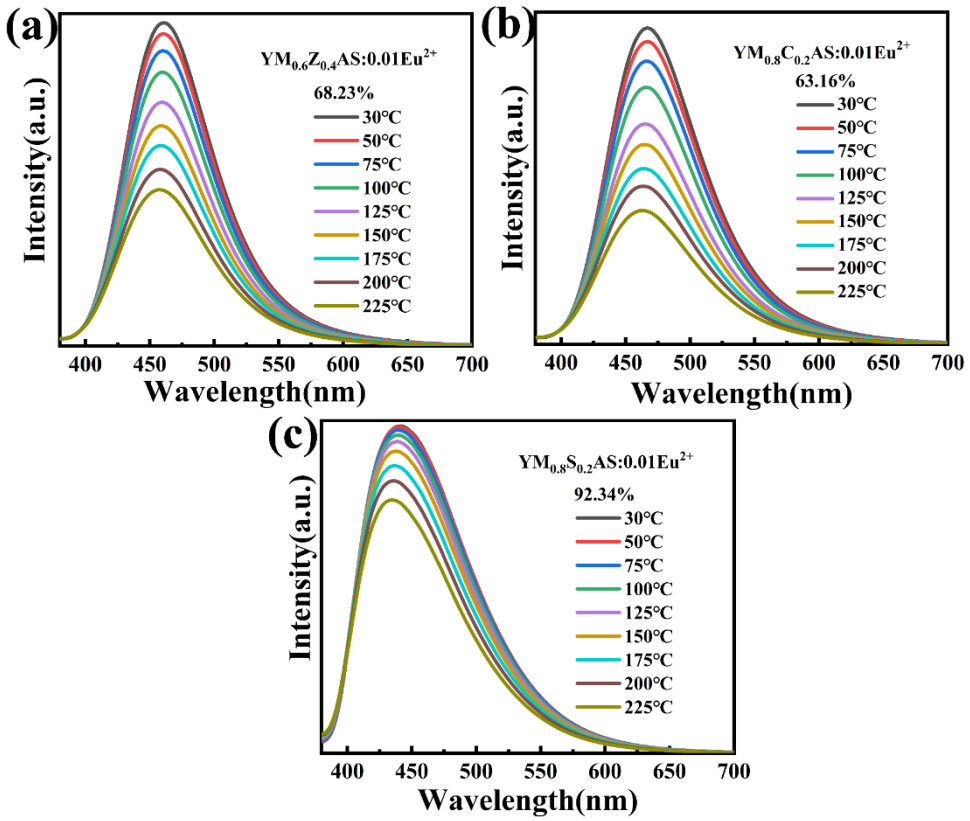

Fig. S10 Temperature spectra of single cation 0.4Zn, 0.2Ca, 0.2Sr substituted for Mg at 365 nm excitation wavelength.

Table S1 Distance from the central atom to the ligand in the octa-ligand

	YMAS	$YMg_{0.6}Zn_{0.4}AS:0.01Eu^{2+}$	$YMg_{0.8}Ca_{0.2}AS:0.01Eu^{2+}$	$YMg_{0.8}Sr_{0.2}AS:0.01Eu^{2+}$
O_1	2.300	2.299	2.300	2.302
O_2	2.300	2.299	2.300	2.302
O_3	2.300	2.299	2.300	2.302
O_4	2.300	2.299	2.300	2.302
O_5	2.429	2.428	2.430	2.431
O_6	2.429	2.428	2.430	2.431
O_7	2.429	2.428	2.430	2.431
O_8	2.429	2.428	2.430	2.431
d_{av}	2.3645	2.3635	2.365	2.3665

Table S2 Distance from the central atom to the ligand in the six coordination

	YMAS	$YMg_{0.6}Zn_{0.4}AS:0.01Eu^{2+}$	$YMg_{0.8}Ca_{0.2}AS:0.01Eu^{2+}$	$YMg_{0.8}Sr_{0.2}AS:0.01Eu^{2+}$
O_1	1.934	1.934	1.935	1.936
O_2	1.934	1.934	1.935	1.936
O_3	1.934	1.934	1.935	1.936
O_4	1.934	1.934	1.935	1.936
O_5	1.934	1.934	1.935	1.936
O_6	1.934	1.934	1.935	1.936
d_{av}	1.934	1.934	1.935	1.936

Table S3 Color purity varies with temperature

T	YMAS: $0.01Eu^{2+}$	$YM_{0.6}Z_{0.4}AS$: $0.01Eu^{2+}$	$YM_{0.8}C_{0.2}AS$: $0.01Eu^{2+}$	$YM_{0.8}S_{0.2}AS$: $0.01Eu^{2+}$
30°	55.12%	73.71%	66.30%	74.22%
50°	55.25%	73.93%	66.62%	74.30%
75°	56.38%	74.27%	66.28%	74.46%
100°	56.71%	74.67%	66.79%	74.76%
125°	57.93%	75.12%	67.48%	74.47%
150°	59.26%	74.69%	68.06%	75.02%
175°	59.96%	75.04%	67.76%	75.72%
200°	60.51%	75.45%	68.29%	75.80%
225°	61.80%	75.83%	68.87%	76.61%