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Crystal field modulation-controlled, bandgap engineering and shallow/deep traps tailoring-guided design of a color-tunable long-persistent phosphor (Ca, Sr)Ga_4O_7:Mn^{2+}, Bi^{3+}

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Table S1. (a) The Wyckoff position, atomic coordinates and occupancies of $CaGa_4O_7$:0.002Mn^{2+}.

Site	Wyckoff position	x	y	z	Occupancy
Ca1	4e	0.0000	0.2970	0.2500	1.0000
Ga1	8f	0.1210	0.0620	0.7430	1.0000
Ga2	8f	0.3400	0.0850	0.1880	1.0000
O1	8f	0.1950	0.0580	0.0750	1.0000
O2	8f	0.3830	0.0680	0.0900	1.0000
O3	8f	0.1160	0.2500	0.3550	1.0000
O4	4e	0.0000	0.0620	0.2500	1.0000

Table S1. (b) The Wyckoff position, atomic coordinates and occupancies of $Sr_{0.3}Ca_{0.7}Ga_4O_7$:0.002Mn^{2+}.

Site	Wyckoff position	x	y	z	Occupancy
Ca1	4e	0.0000	0.2970	0.2500	0.7000
Ga1	8f	0.1210	0.0620	0.7430	1.0000
Ga2	8f	0.3400	0.0850	0.1880	1.0000
O1	8f	0.1950	0.0580	0.0750	1.0000
O2	8f	0.3830	0.0680	0.0900	1.0000
O3	8f	0.1160	0.2500	0.3550	1.0000
O4	4e	0.0000	0.0620	0.2500	1.0000
Sr1	4e	0.0000	0.2970	0.2500	0.3000

Table S1 (c) The Wyckoff position, atomic coordinates and occupancies of $Sr_{0.5}Ca_{0.5}Ga_4O_7$:0.002Mn^{2+}.

Site	Wyckoff position	x	y	z	Occupancy
Ca1	4e	0.0000	0.2970	0.2500	0.5000
Ga1	8f	0.1210	0.0620	0.7430	1.0000
Ga2	8f	0.3400	0.0850	0.1880	1.0000
O1	8f	0.1950	0.0580	0.0750	1.0000
O2	8f	0.3830	0.0680	0.0900	1.0000
O3	8f	0.1160	0.2500	0.3550	1.0000
O4	4e	0.0000	0.0620	0.2500	1.0000
Sr1	4e	0.0000	0.2970	0.2500	0.5000

Table S1. (d) The Wyckoff position, atomic coordinates and occupancies of $Sr_{0.8}Ca_{0.2}Ga_4O_7$:0.002Mn^{2+}.

Site	Wyckoff position	x	y	z	Occupancy
Ca1	4e	0.0000	0.3120	0.2500	0.2000
Ga1	8f	0.3804	0.4408	0.2417	1.0000
Ga2	8f	0.3318	0.0863	0.2020	1.0000
O1	8f	0.1900	0.0630	0.0880	1.0000
O2	8f	0.1150	0.4490	0.0580	1.0000
O3	8f	0.3810	0.2500	0.3520	1.0000
O4	4e	0.0000	0.0360	0.2500	1.0000
Sr1	4e	0.0000	0.3120	0.2500	0.8000

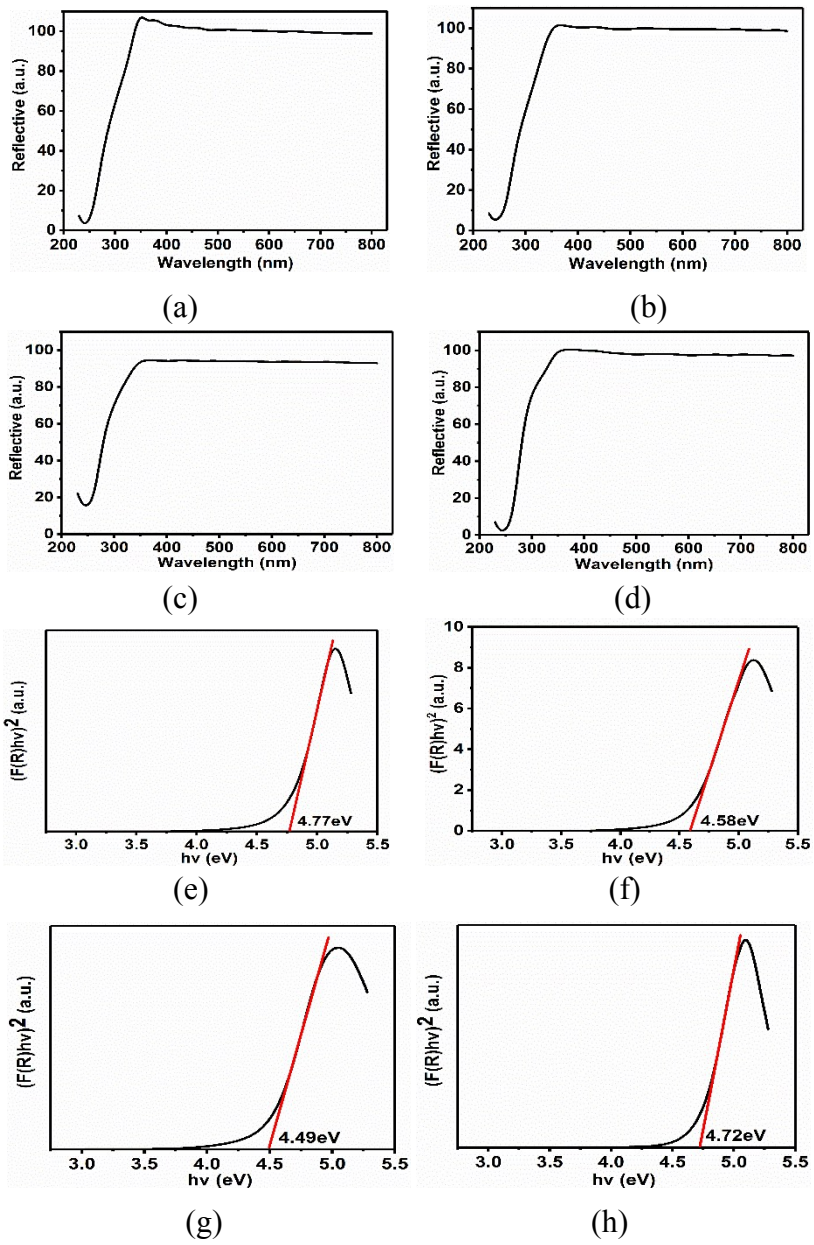


Fig. S1. Diffuse reflectance spectra of (a) $CaGa_4O_7$, (b) $Sr_{0.3}Ca_{0.7}Ga_4O_7$, (c) $Sr_{0.5}Ca_{0.5}Ga_4O_7$, (d) $Sr_{0.8}Ca_{0.2}Ga_4O_7$; $[F(R)h\nu]^2$ vs. photon energy hν of (a) $CaGa_4O_7$, (b) $Sr_{0.3}Ca_{0.7}Ga_4O_7$, (c) $Sr_{0.5}Ca_{0.5}Ga_4O_7$, (d) $Sr_{0.8}Ca_{0.2}Ga_4O_7$.

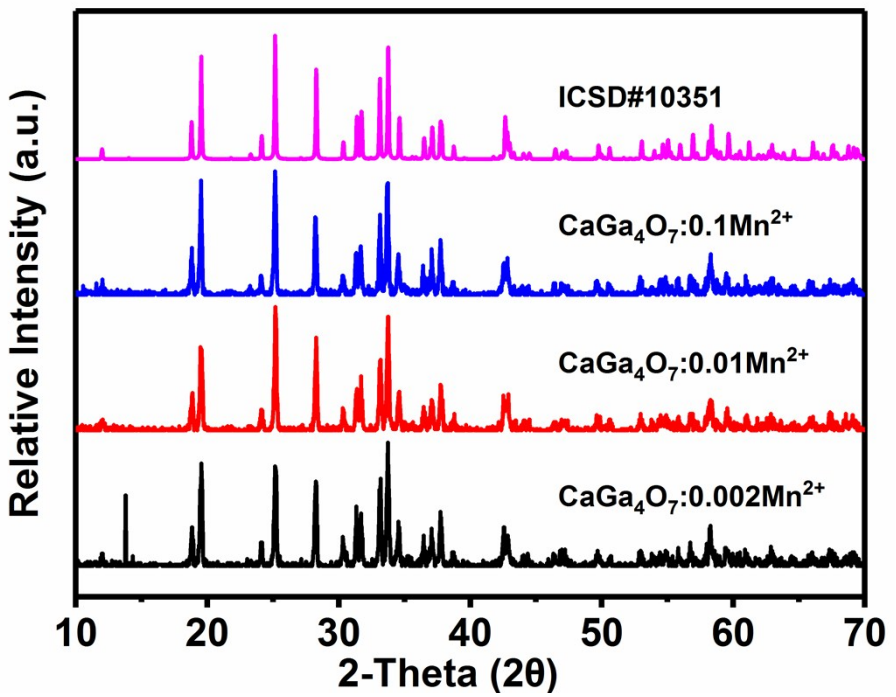
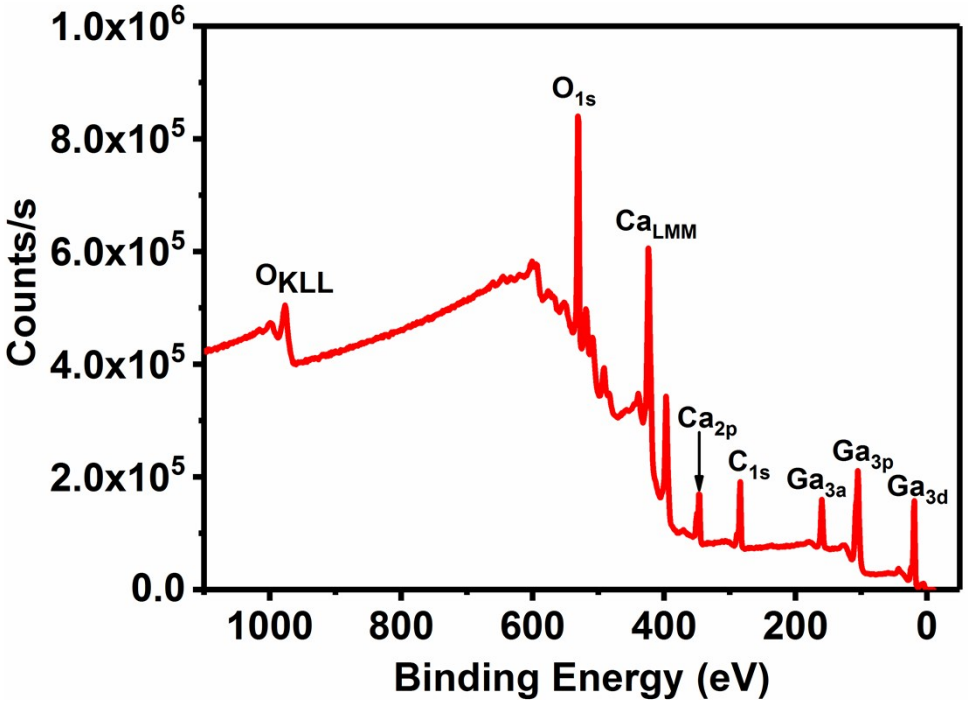
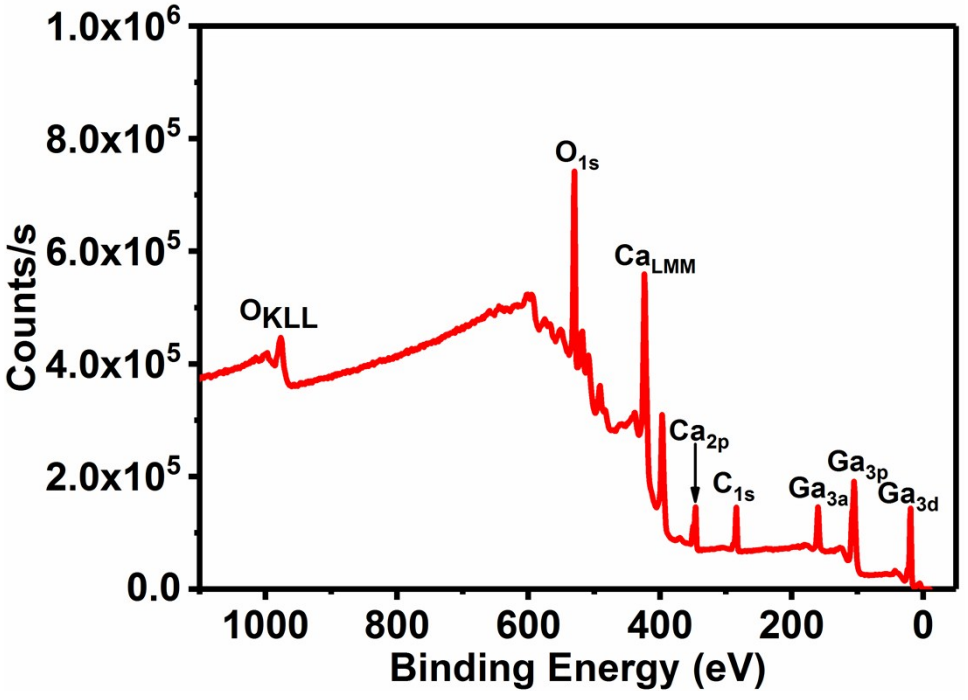


Fig. S2. XRD patterns of $CaGa_4O_7:yMn^{2+}$ (y=0.002, 0.01, and 0.1) and the comparison with ICSD#10351 for $CaGa_4O_7$.



(a)



(b)

Fig. S3. (a)The XPS of $CaGa_4O_7$:0.01Mn^{2+} (the starting materials $MnCO_3$ was used as Mn sources). (b) The XPS of $CaGa_4O_7$:0.1Mn^{2+} (the starting materials MnO_2 was used as Mn sources).

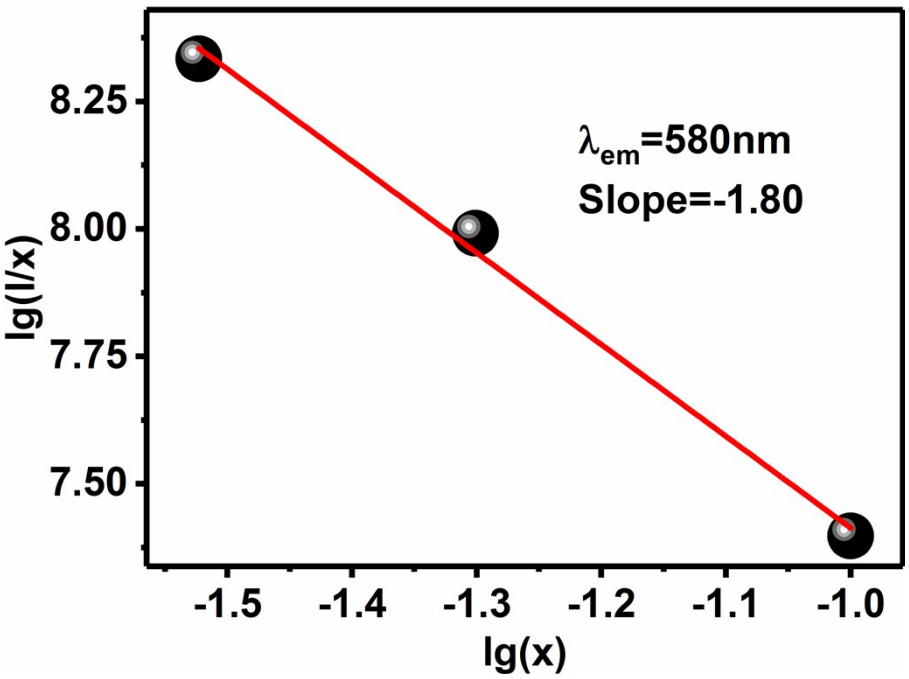


Fig. S4. The dependence of lg(I/x) on lg(x) according to Eq. (3).

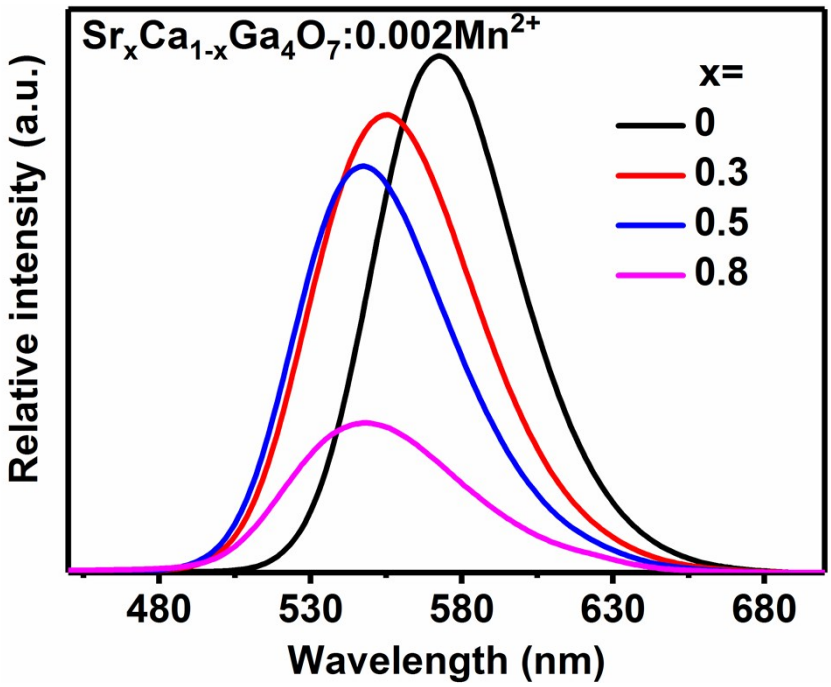


Fig. S5. The LPL spectra of samples $Sr_xCa_{1-x}Ga_4O_7$:0.002Mn^{2+} immediately measured after 254 nm irradiation for 5 min.

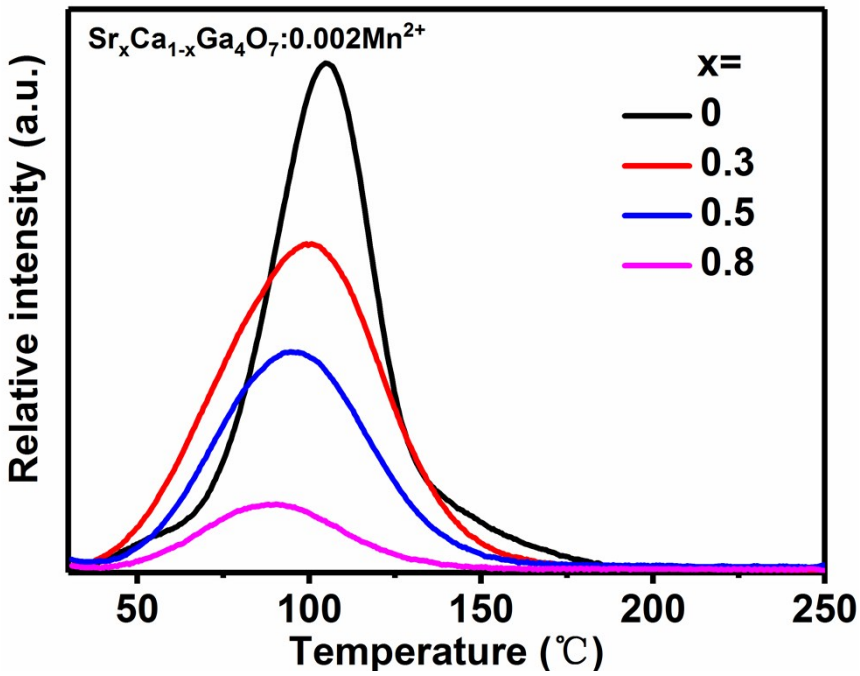


Fig. S6. TL glow curves of $Sr_xCa_{1-x}Ga_4O_7$:0.002Mn^{2+} (x=0, 0.3, 0.5, 0.8) measured 3 min after irradiation with UV light (250 nm) for 5 min.

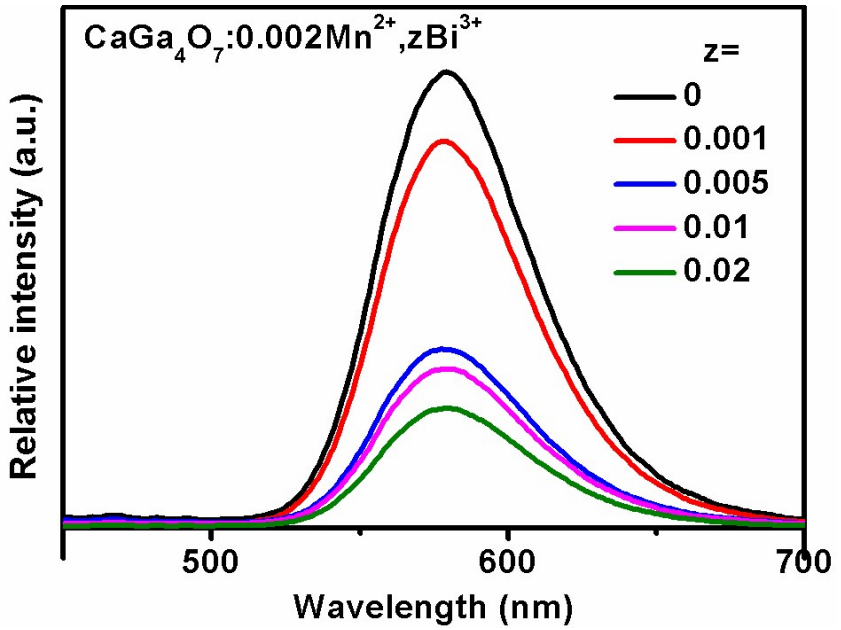


Fig. S7. The emission spectra of $CaGa_4O_7$:0.002Mn^{2+}, zBi^{3+} (z=0, 0.001, 0.005, 0.01, 0.02).

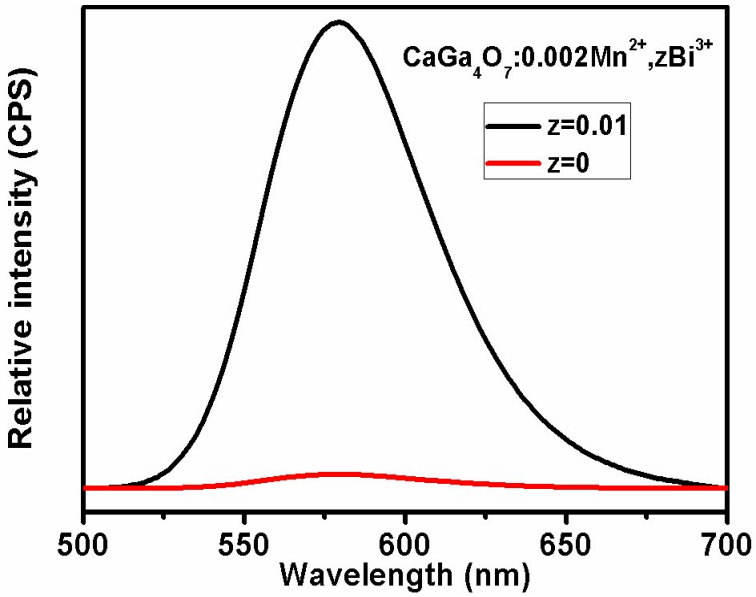


Fig. S8. LPL spectra of samples $CaGa_4O_7$:0.002Mn^{2+}, zBi^{3+} (z=0 and 0.01) recorded immediately after UV irradiation.