Supporting information

Key Role of Metal-to-Metal Charge Transfer Transition between Mo^{6+} and Bi^{3+} for Enhancement in NIR Luminescence of Gd_2MoO_6:Bi,Yb Nanophosphor

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Figure and Table content

Table S7. Fitting parameters of decay curves for GMO:Bi,*y*Yb (*y* = 0, 0.5, and 1 mol%) nanophosphors measured at 77 K (λ_{ex}= 360 nm and λ_{em}= 670 nm).

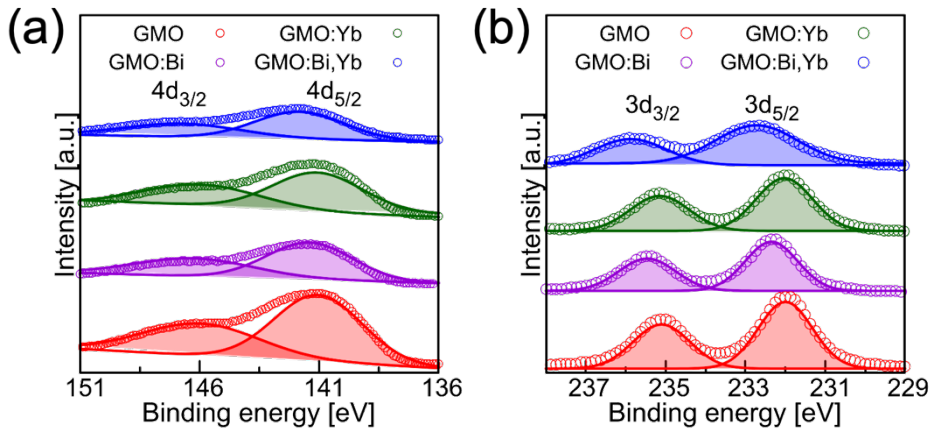

Figure S1. Narrow scan analysis of XPS for (a) Gd 4d and (b) Mo 3d.

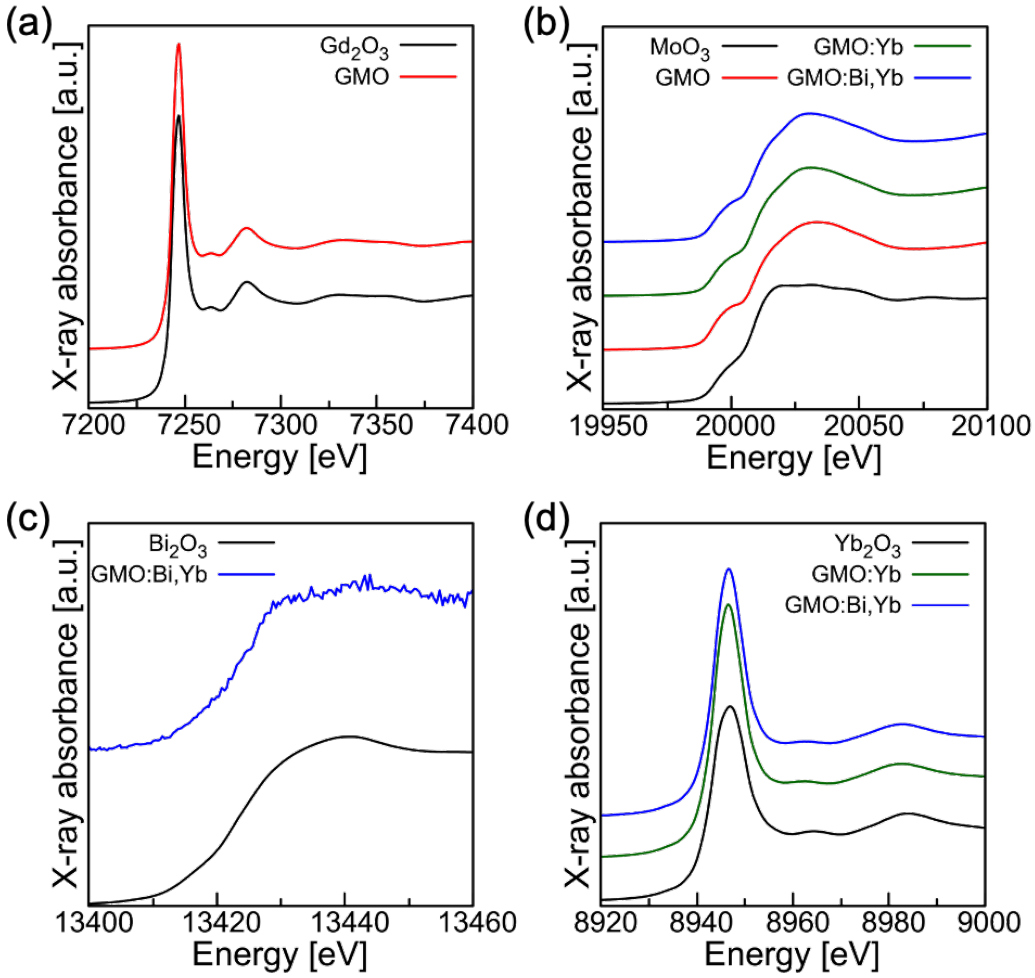

Figure S2. XANES spectra for all GMO nanophosphors of (a) Gd L_3-, (b) Mo K-, (c) Bi L_3-, and (d) Yb L_3-edge with the reference samples (Gd_2O_3, MoO_3, Bi_2O_3, and Yb_2O_3).

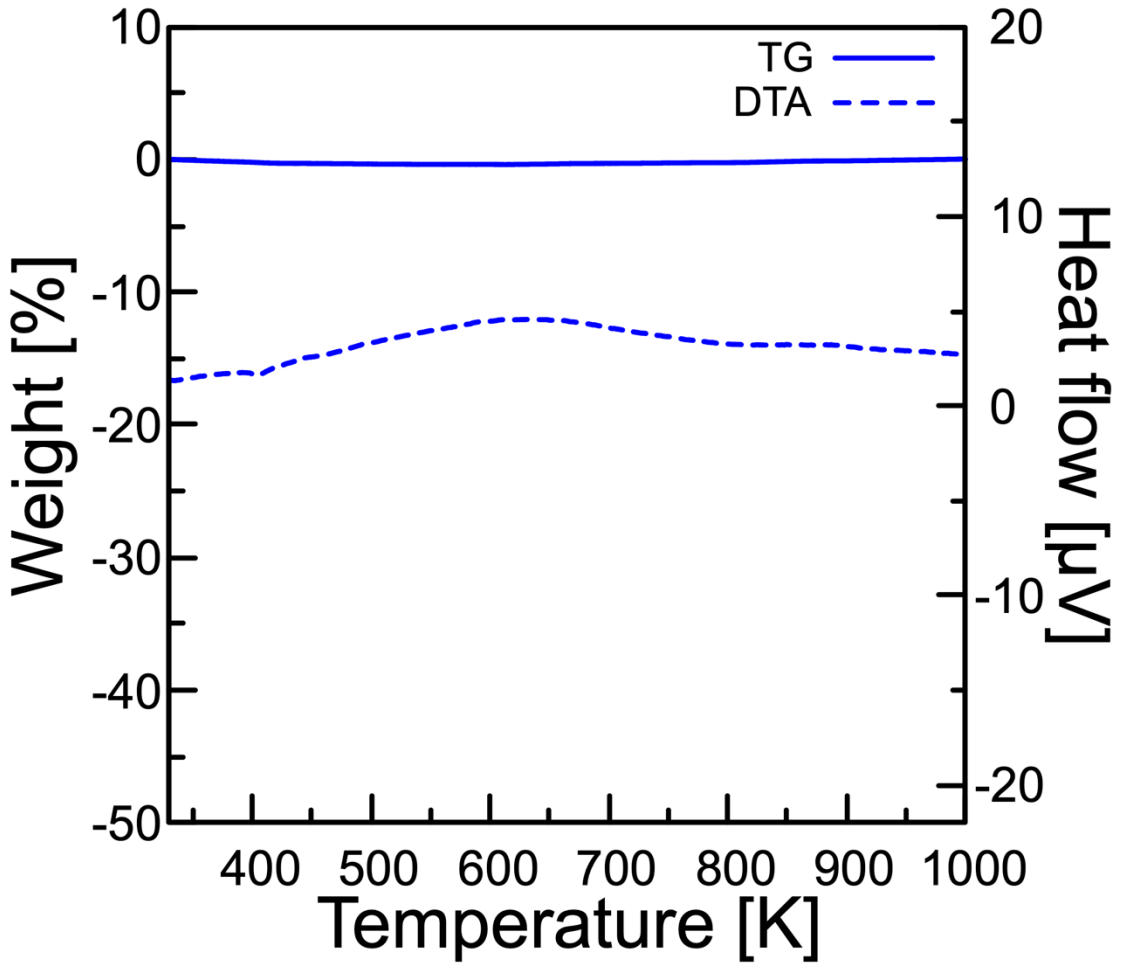

Figure S3. TG-DTA curve for GMO:Bi,Yb, and from 330 K to 1000 K under ambient air.

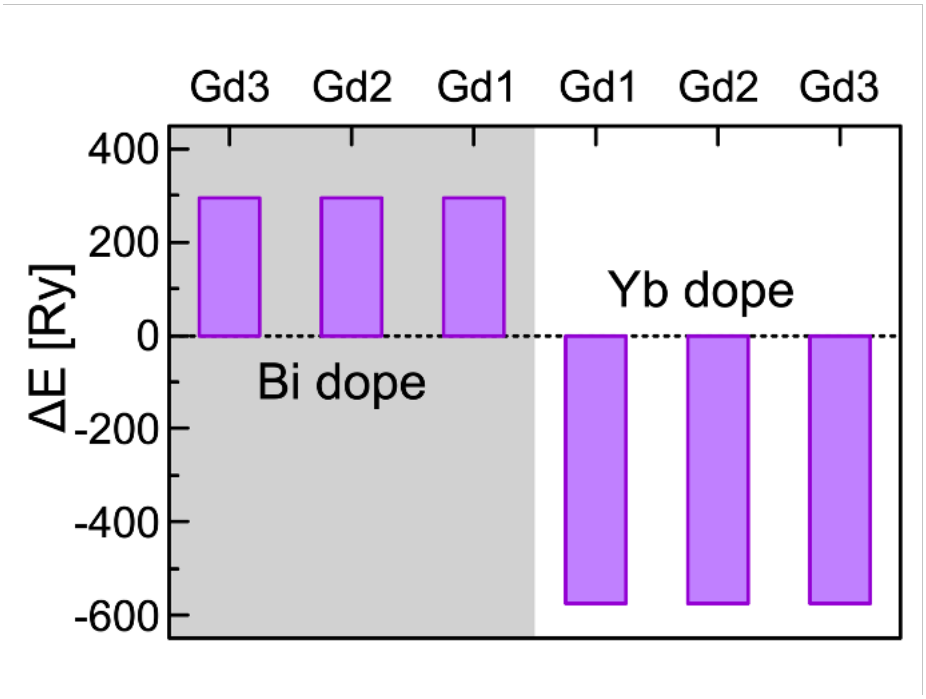

Figure S4. Δ*E* values calculated from the total energy obtained after structural relaxation.

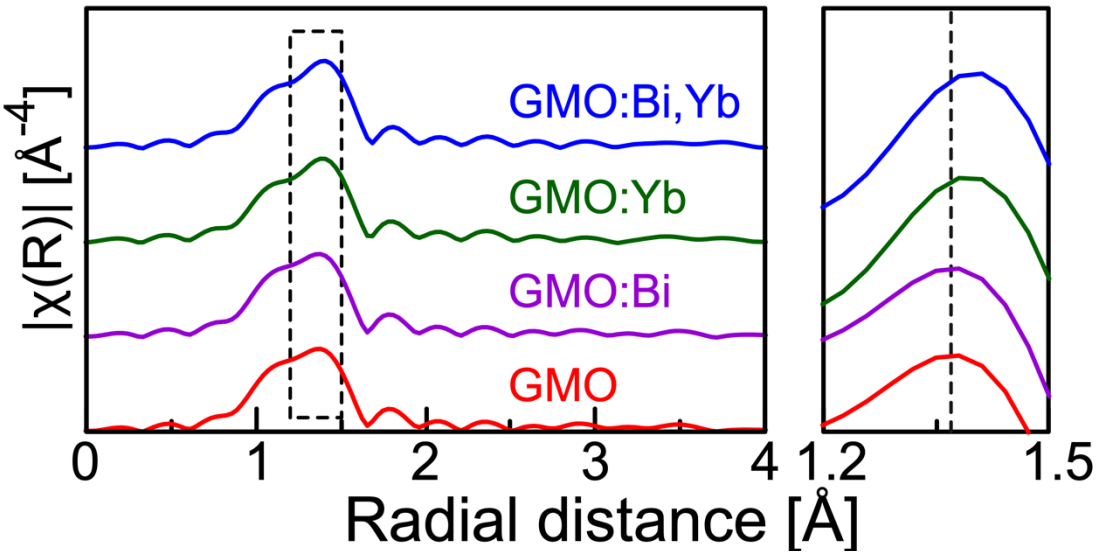

Figure S5. Fourier transformed EXAFS radial distribution function spectra of Mo *K*-edge in all GMO nanophosphors.

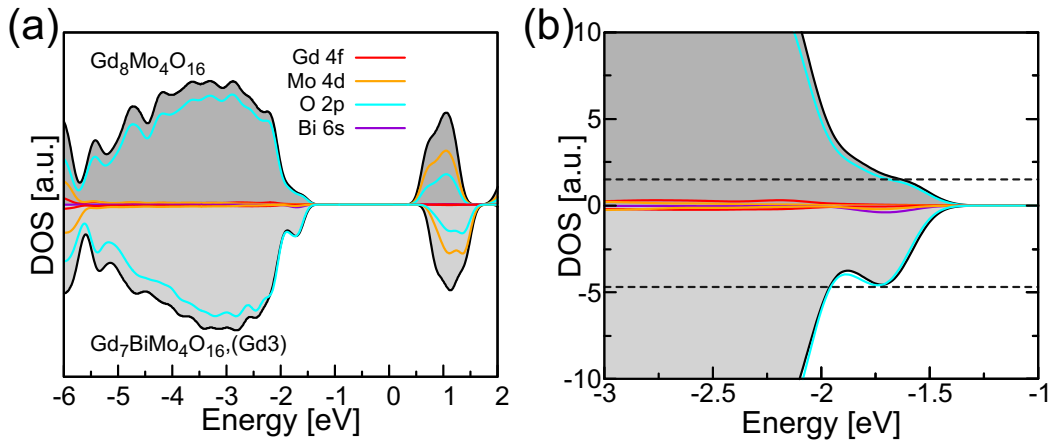

Figure S6. (a) DOS/pDOS of GMO:Bi substituted in Gd3 site, and (b) enlarged one.

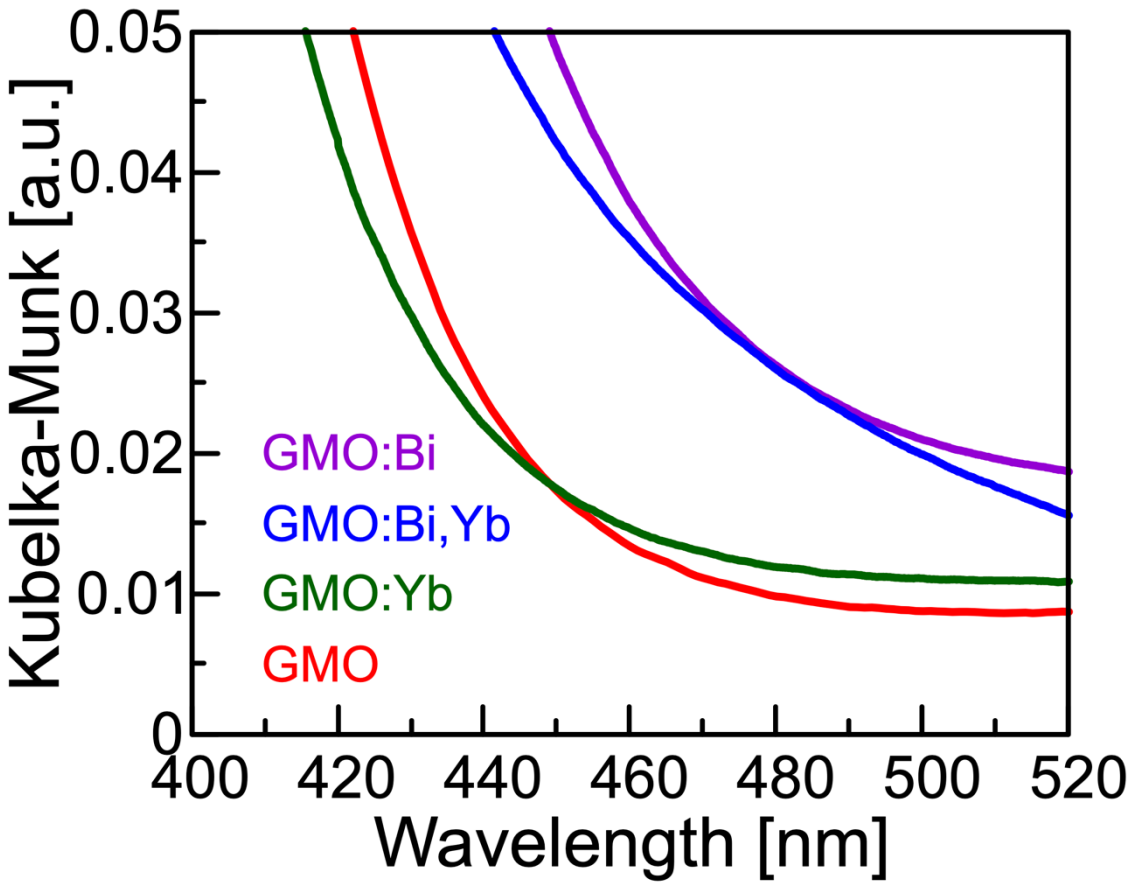

Figure S7. Kubelka-Munk spectra of all GMO nanophosphors around 500 nm.

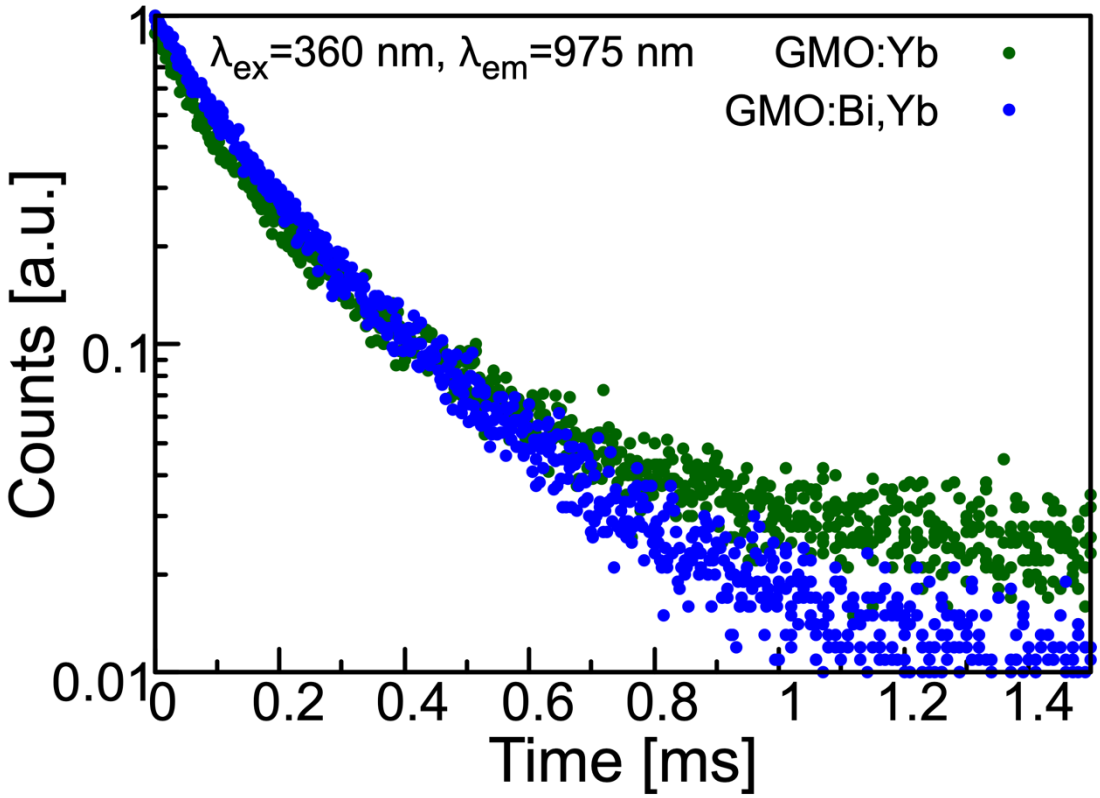

Figure S8. Decay curves of GMO:Yb and GMO:Bi,Yb at 300 K (λ_{ex}= 360 nm and λ_{em}= 975 nm).

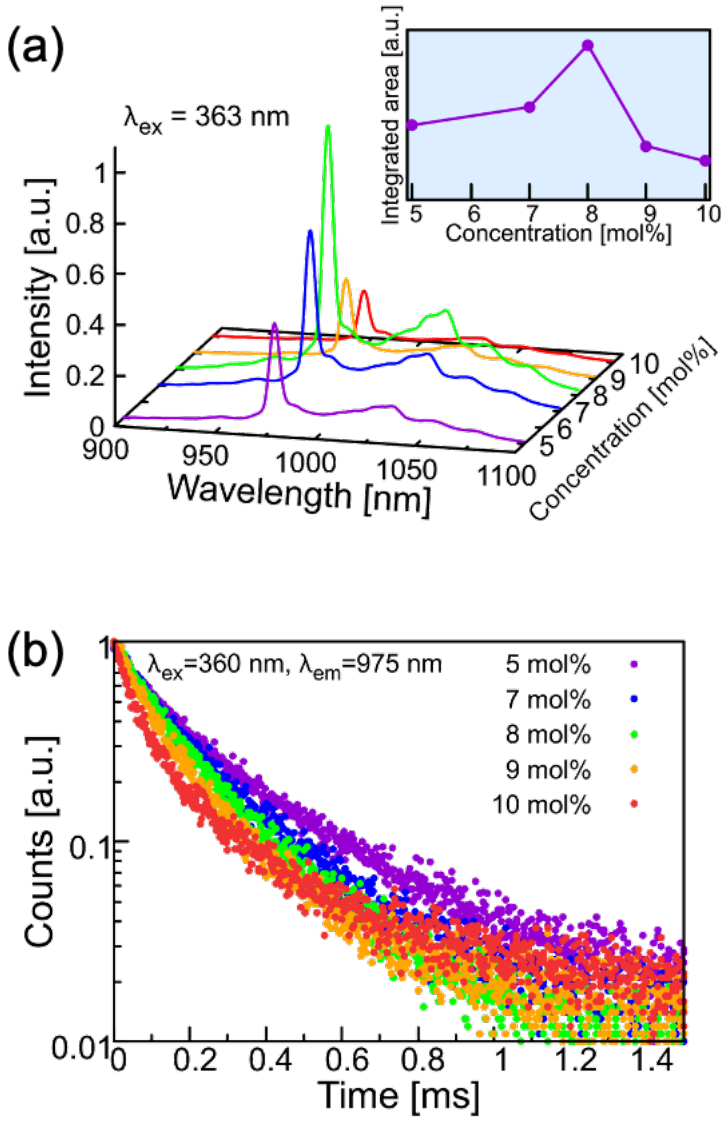

Figure S9. (a) PL spectra (λ_{ex}= 363 nm) and (b) decay curve (λ_{ex}= 360 nm and λ_{em}= 975 nm) of GMO:Bi,yYb (y = 5, 7, 8, 9, and 10 mol%) nanophosphors at 300 K.

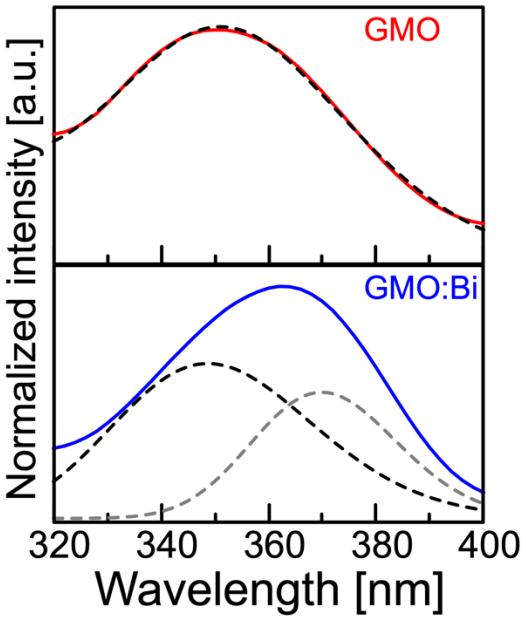

Figure S10. Gaussian fit of PLE spectra for GMO and GMO:Bi at 77 K.

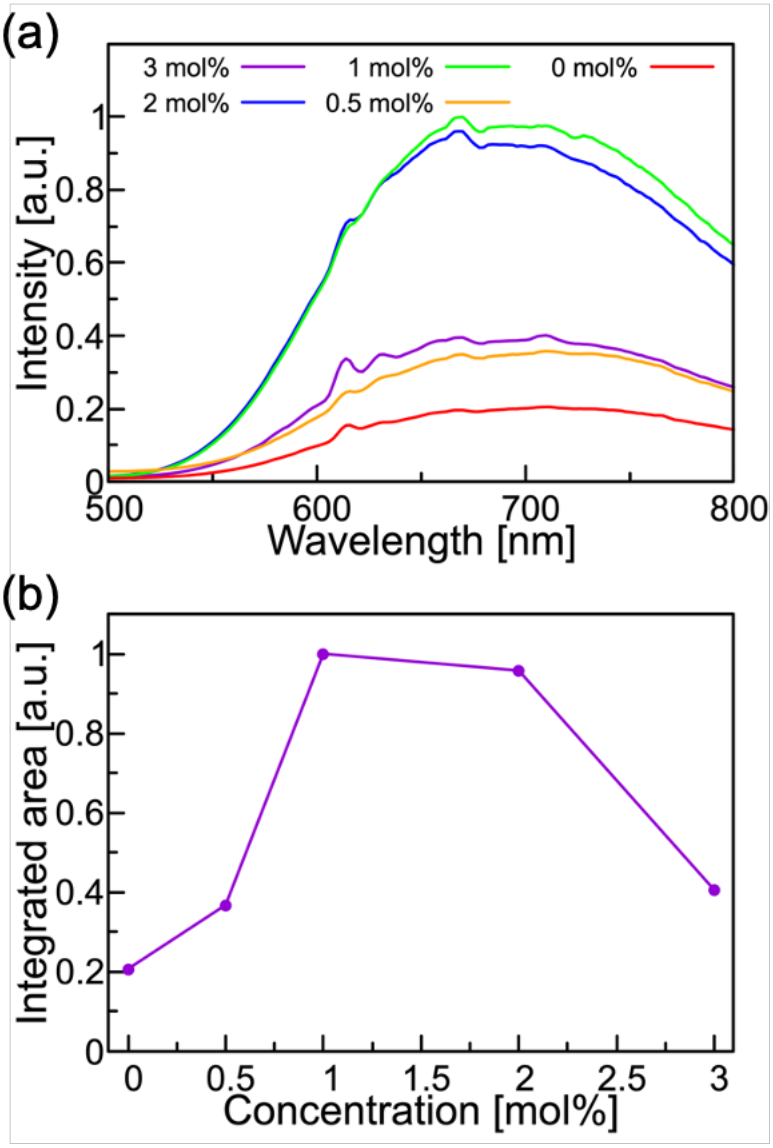

Figure S11. (a) PL spectra (λ_{ex}= 360 nm) and (b) integrated intensity of GMO:*x*Bi, (*x* = 0, 0.5, 1, 2, and 3 mol%) nanophosphors at 77 K.

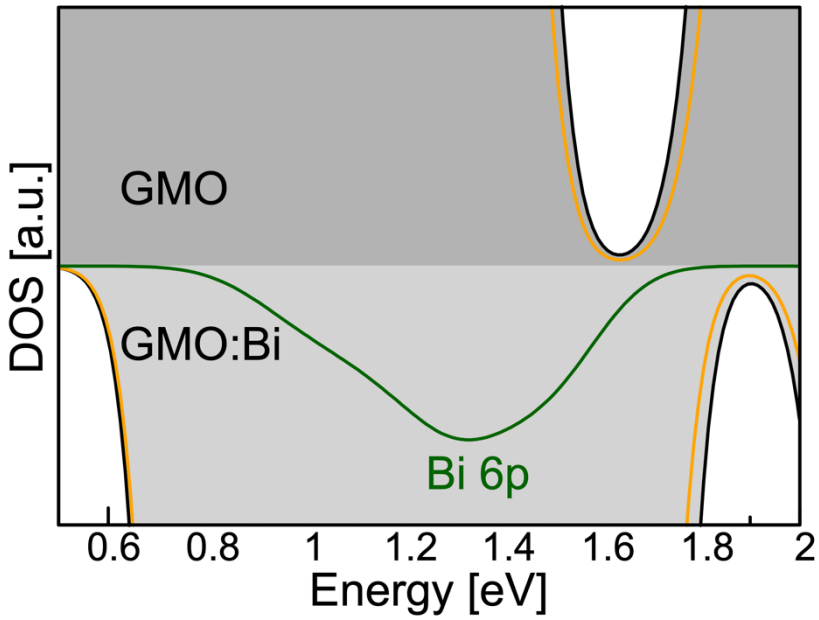

Figure S12. Enlarged DOS/pDOS of GMO:Bi substituted in Gd1 around conduction band minimum.

Table S1. Molar ratios of Gd/Bi/Yb for all GMO nanophosphors calculated from XPS.

	GMO	GMO:Bi	GMO:Yb	GMO:Bi,Yb
Gd [mol%]	100	94.6	96.2	90.4
Bi [mol%]	0	5.33	-	7.92
Yb [mol%]	0	-	3.80	1.67

Table S2 Lattice parameters for each GMO nanophosphor refined by Rietveld analysis.

	GMO	GMO:Bi	GMO:Yb	GMO:Bi,Yb
a [Å]	16.54(1)	17.13(1)	17.13(1)	16.508(4)
b [Å]	11.183(6)	10.796(4)	10.741(5)	11.161(3)
c [Å]	5.408(3)	5.417(5)	5.395(2)	5.394(1)
β [°]	108.50(3)	108.50(7)	108.50(3)	108.247(1)
V [Å^3]	949(1)	950(1)	941.2(8)	942.7(4)
R_{wp} [%]	9.788	10.48	8.252	9.133
R_p [%]	7.463	7.710	6.234	7.218
S	3.013	2.727	1.729	2.231

Table S3. Lattice parameters and average bond length for each GMO nanophosphor refined by Rietveld analysis.

		CIF	DFT	Rietveld
Lattice parameter	*a* [Å]	9.959	9.904	10.004
	b [Å]	9.959	9.903	10.004
	c [Å]	5.418	5.393	5.412
	α [°]	105.06	104.78	105.25
	β [°]	105.06	104.79	105.25
	γ [°]	68.223	68.292	67.877
Average bond length	Gd1-O	2.449	2.430	2.451
	Gd2-O	2.442	2.417	2.425
	Gd3-O	2.405	2.395	2.406
	Mo-O	1.884	1.876	1.896

Table S4. Calculated total energy after structural relaxation and ΔE values.

		Total energy [Ry]	ΔE [Ry]
GMO		-11949.258	-
Bi	Gd1	-11653.825	295.433
	Gd2	-11653.826	295.432
	Gd3	-11653.837	295.421
Yb	Gd1	-12525.176	-575.918
	Gd2	-12525.160	-575.902
	Gd3	-12525.160	-575.902

Table S5. Fitting parameters of decay curves for GMO:Yb and GMO:Bi,Yb measured at 300 K.

Sample	τ_1 [μs]	τ_2 [μs]	A_1 [-]	A_1 [-]	τ_{ave} [μs]
GMO:Yb	58.3	239	461	454	203
GMO:Bi,Yb	97.3	265	583	410	207

Table S6. Fitting parameters of decay curves for GMO:Bi,*y*Yb (*y*= 5, 7, 8, 9, and 10 mol%) measured at 300 K.

y [mol%]	τ_1 [μs]	τ_2 [μs]	A_1 [-]	A_2 [-]	τ_{ave} [μs]
5	95.3	340	441	496	291
7	102	299	557	420	238
8	97.3	265	583	410	207
9	73.4	229	611	402	178
10	50.1	265	674	302	201

Table S7. Fitting parameters of decay curves for GMO:Bi,*y*Yb (*y* = 0, 0.5, and 1 mol%) nanophosphors measured at 77 K (λ_{ex}= 360 nm and λ_{em}= 670 nm).

y [mol%]	τ_1 [μs]	τ_2 [μs]	A_1 [-]	A_2 [-]	τ_{ave} [μs]
0	6.61	34.3	0.0240	0.00378	19.1
0.5	3.11	28.8	0.0322	0.00305	15.1
1	2.28	23.2	0.0375	0.00290	11.5