Supporting Information

Luminescence Tuning of NIR Luminescence Nanophosphor Bi^{3+}/Yb^{3+}-doped RE_2MoO_6 (RE=Gd, Y, Lu) and $Gd_2Mo_{1-x}W_xO_6$

Taisei Hangai,[1] Takuya Hasegawa,*[,1] Jian Xu,[2] Takayuki Nakanishi,[3] Takashi Takeda,[3] Tomoyo Goto,[4,5] Yasushi Sato,[6] Ayahisa Okawa,[1] and Shu Yin[1,7]

[1] Institute of Multidisciplinary Research for Advanced Material (IMRAM), Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577, Japan

[2] International Center for Young Scientists (ICYS), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0044, Japan

[3] Advanced Phosphor Group, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, 305-0044, Japan

[4] SANKEN (The Institute of Scientific and Industrial Research), Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan

[5] Institute for Advanced Co-Creation Studies, Osaka University, 1-1 Yamadaoka, Suita, Osaka, 565-0871, Japan

[6] Department of Chemistry, Faculty of Science, Okayama University of Science, 1-1 Ridai-cho, Kita-ku, Okayama 700-0005, Japan

[7] Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan

*Corresponding author:
Takuya Hasegawa: hase@tohoku.ac.jp

Figure and Table content

Figure S1. Narrow scan analysis of (a) Gd 4d, (b) Y 3d, (c) Lu 3d, (d) Mo 3d, (e) Bi 4f, and (f) Yb 4d for REMO:Bi,Yb nanophosphors (RE=Gd, Y, and Lu).

Figure S2. XANES spectra for REMO:Bi,Yb (RE=Gd, Y, and Lu) with the reference samples of MoO_3 and MoO_2.

Figure S3. Derivative XANES spectra for REMO:Bi,Yb (RE=Gd, Y, and Lu) with the reference samples of MoO_3 and MoO_2.

Figure S4. Rietveld analysis for RE_2MoO_6:Bi,Yb (RE = Y(a) and Lu(b)).

Figure S5. Rietveld analysis for RE_2MoO_6 (RE = Gd (a), Y (b) and Lu (c)).

Figure S6. Tauc plot for RE_2MoO_6 (RE = Gd, Y, and Lu).

Figure S7. Fourier transformed EXAFS radial distribution function spectra of Mo K-edge in REMO:Bi,Yb (RE= Gd, Y, and Lu).

Figure S8. Normalized PL spectra in NIR region for REMO:Bi,Yb (RE=Gd, Y, and Lu) under 363 nm excitation.

Figure S9. Temperature-dependent PL spectra in NIR region under 363 nm excitation from 80 K to 300 K for (a) GMO:Bi,Yb, (b) YMO:Bi,Yb, and (c) LuMO:Bi,Yb.

Figure S10. Derivative XANES spectra of Mo K- and W L_3-edge with reference samples of MoO_3, MoO_2, WO_3, and WO_2 for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb.

Figure S11. Normalized PL spectra under 363 nm excitation for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb (x=0, 0.2, and 0.5).

Figure S12. Photographs of PDMS/GMO:Bi,Yb film.

Table S1. Molar ratios of RE/Bi/Yb for REMO:Bi,Yb (RE=Gd, Y, and Lu) estimated from XPS.

Table S2. Lattice parameters for REMO:Bi,Yb (RE=Gd, Y, and Lu) refined by Rietveld analysis.

Table S3. Lattice parameters for REMO (RE=Gd, Y, and Lu) refined by Rietveld analysis.

Table S4. Fitting parameter of decay curves for REMO:Bi,Yb (RE=Gd, Y, and Lu).

Table S5. Fitting parameter of decay curves for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb.
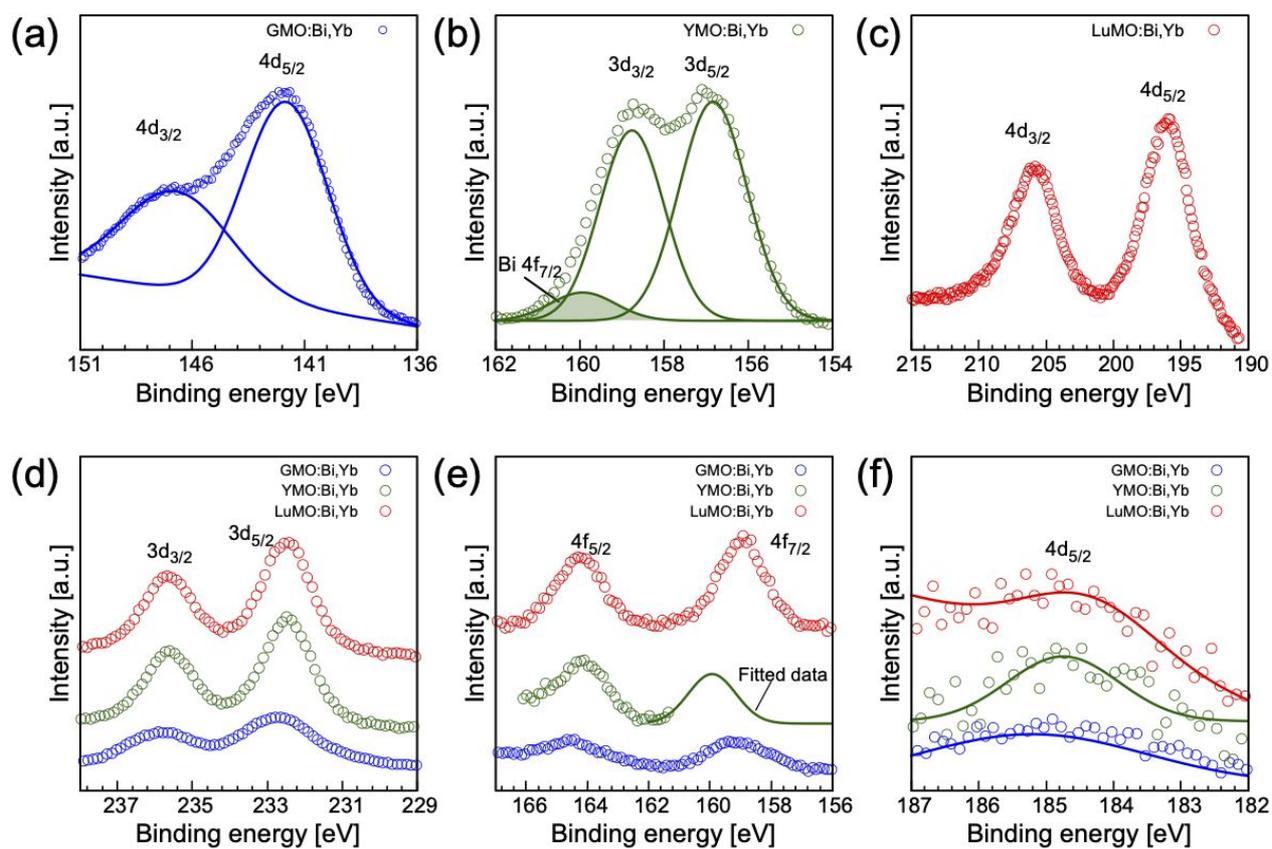
Figure S1. Narrow scan analysis of (a) Gd 4d, (b) Y 3d, (c) Lu 3d, (d) Mo 3d, (e) Bi 4f, and (f) Yb 4d for REMO:Bi,Yb nanophosphors (RE=Gd, Y, and Lu).
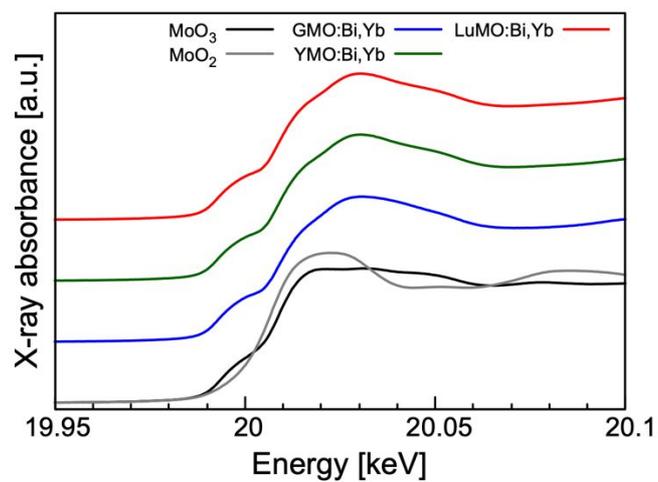
Figure S2. XANES spectra for REMO:Bi,Yb (RE=Gd, Y, and Lu) with the reference samples of MoO_3 and MoO_2.
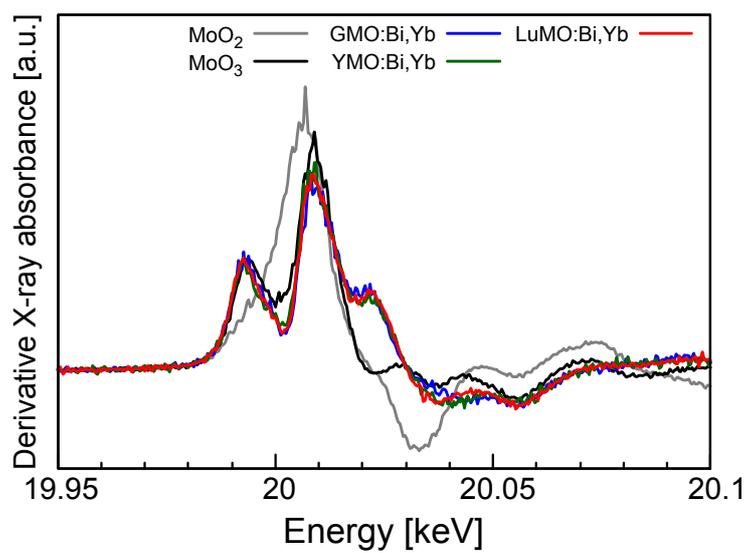
Figure S3. Derivative XANES spectra for REMO:Bi,Yb (RE=Gd, Y, and Lu) with the reference samples of MoO₃ and MoO₂.
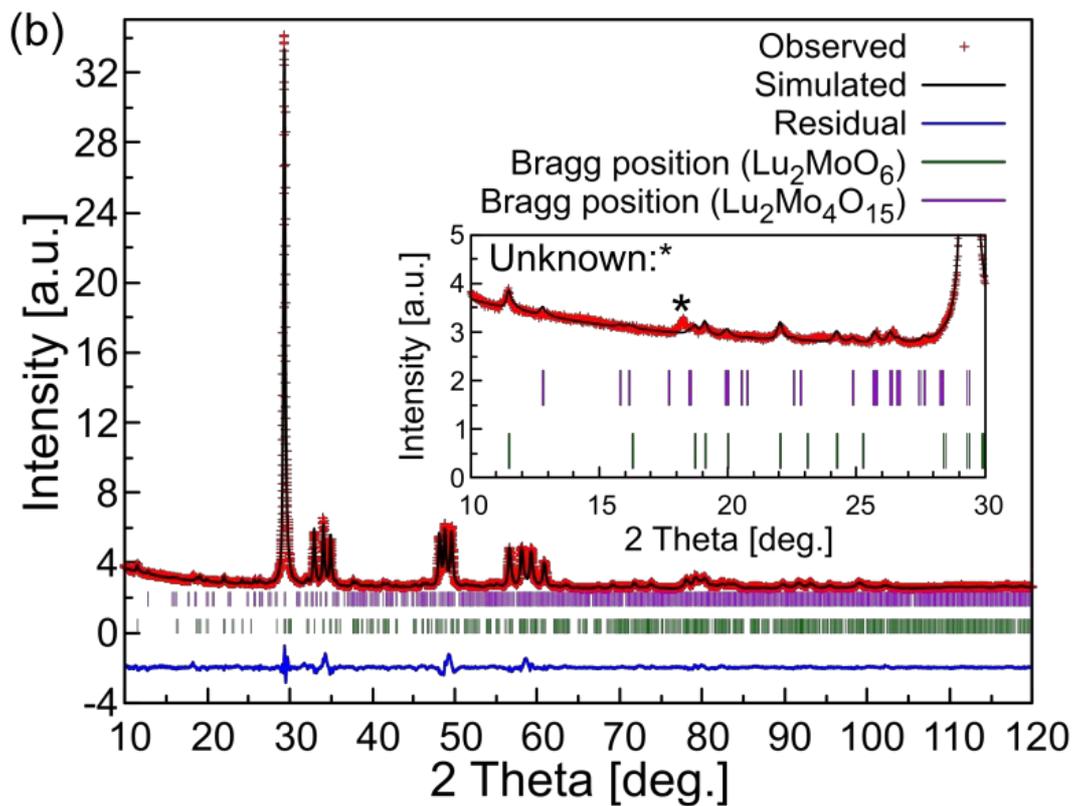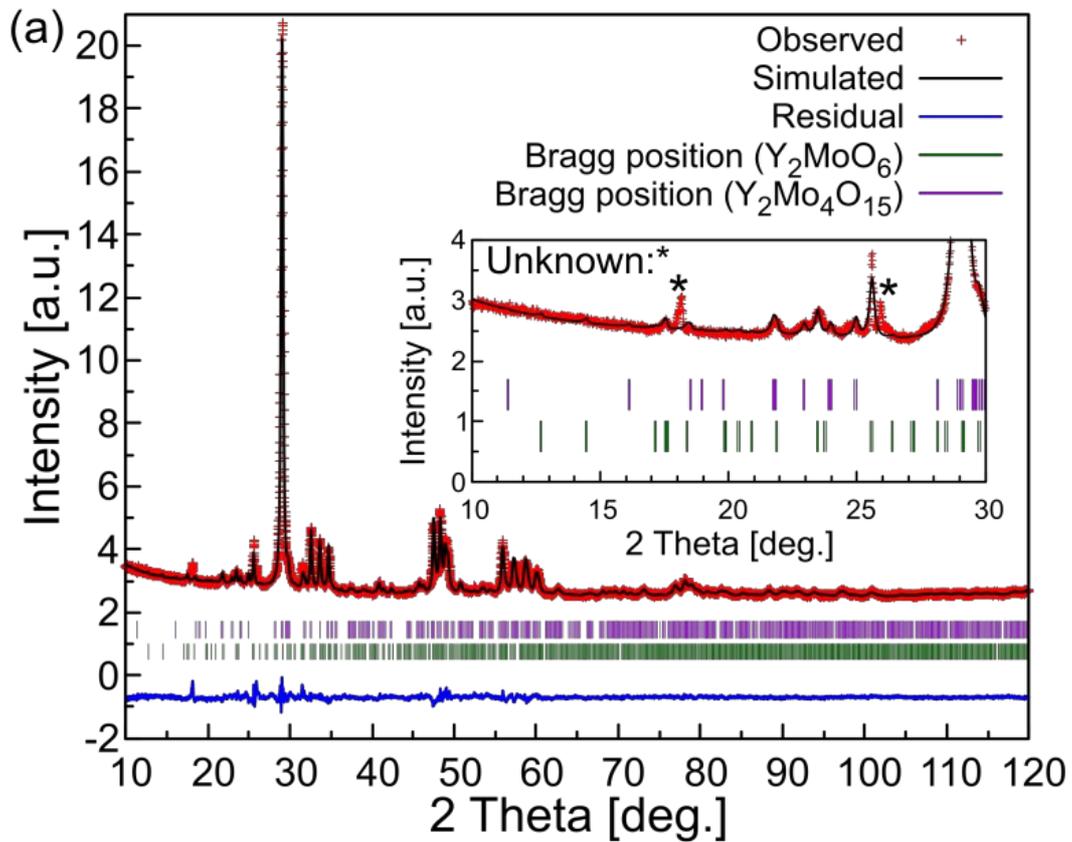
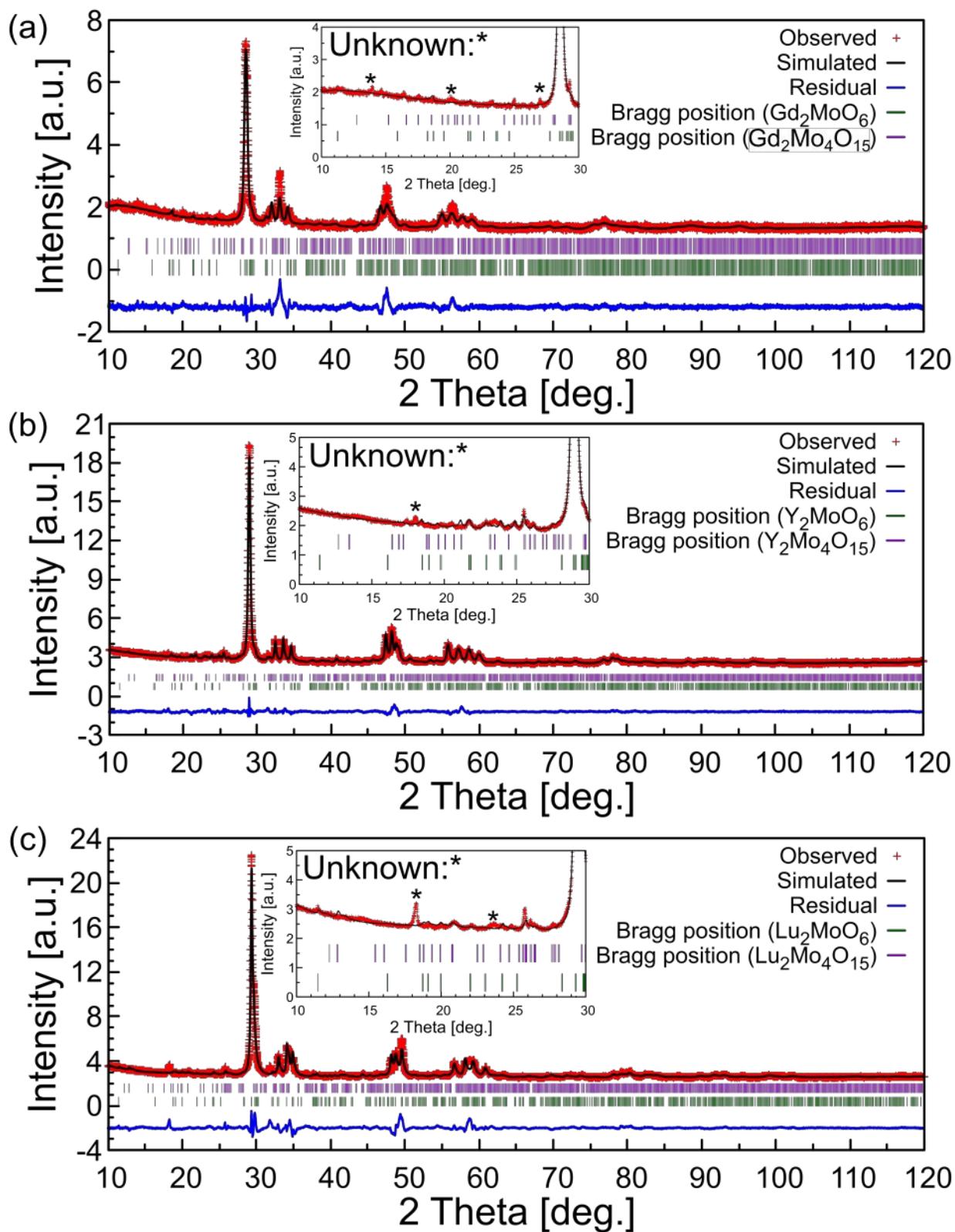Figure S4. Rietveld analysis for REMO:Bi,Yb (RE =Y (a) and Lu (b)).

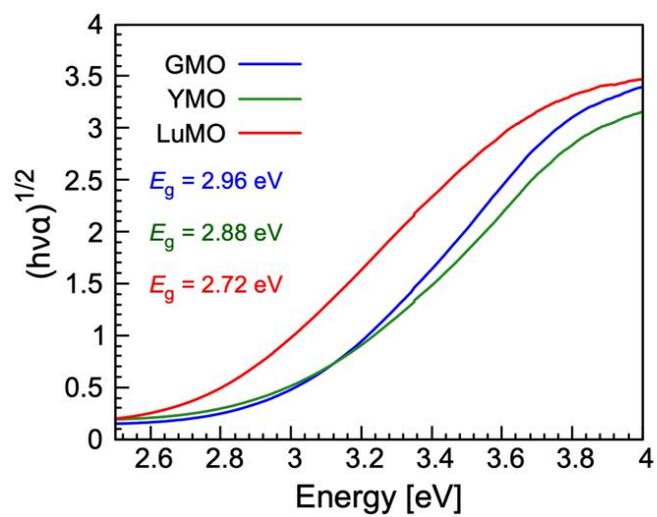Figure S5. Rietveld analysis for REMO (RE =Gd (a), Y (b), and Lu (c)).

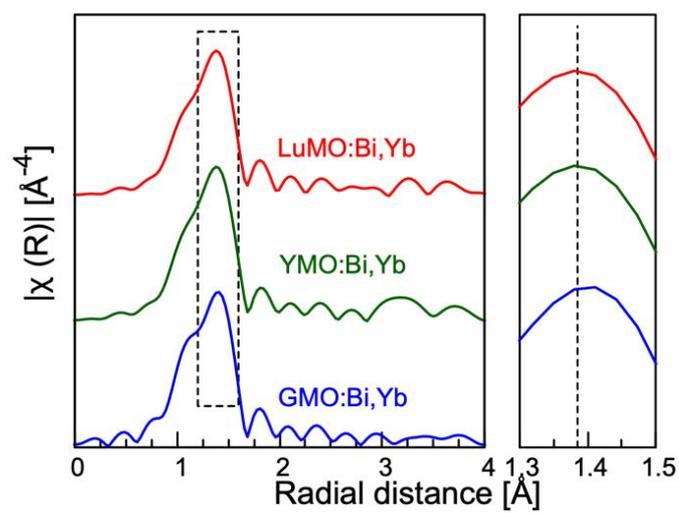Figure S6. Tauc plot for RE$_2$MoO$_6$ (RE = Gd, Y, and Lu).

Figure S7. Fourier transformed EXAFS radial distribution function spectra of Mo K-edge in REMO:Bi,Yb (RE= Gd, Y, and Lu).
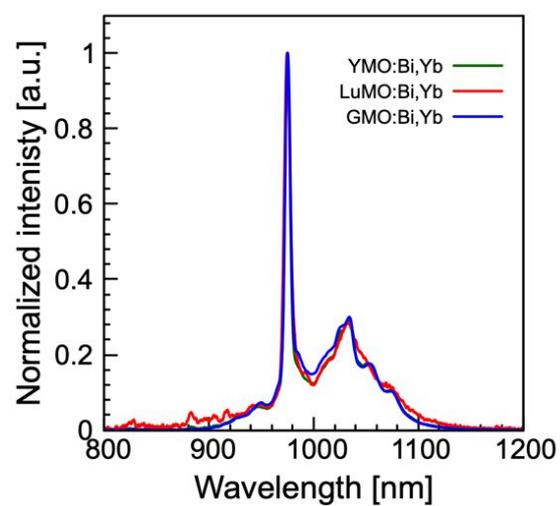
Figure S8. Normalized PL spectra in NIR region for REMO:Bi,Yb nanophosphors (RE=Gd, Y, and Lu) under 363 nm excitation.
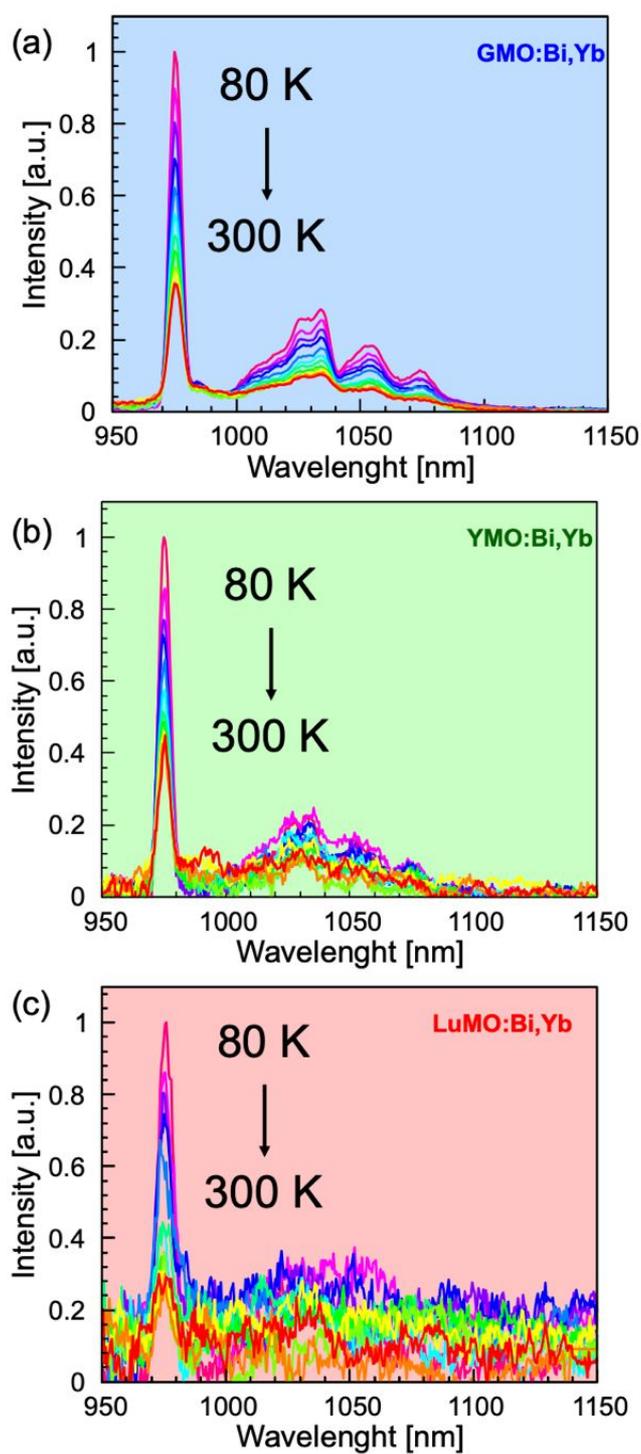
Figure S9. Temperature-dependent PL spectra in NIR region under 363 nm excitation from 80 K to 300 K for (a) GMO:Bi,Yb, (b) YMO:Bi,Yb, and (c) LuMO:Bi,Yb.
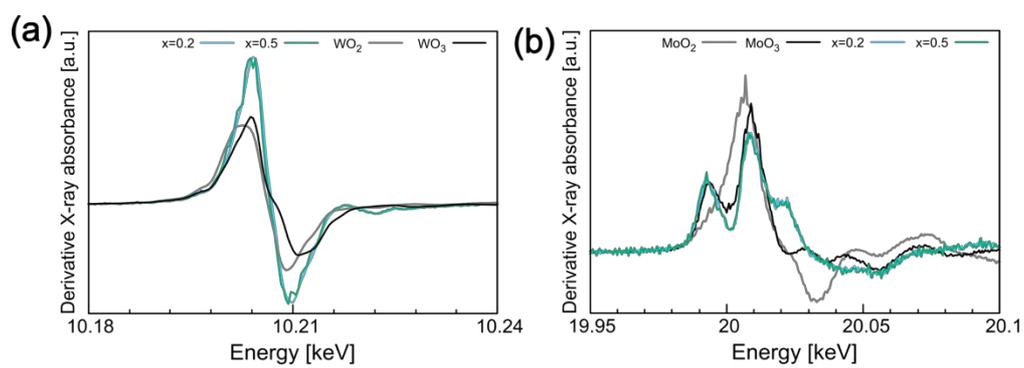
Figure S10. Derivative XANES spectra of Mo K- and W L_3-edge with reference samples of MoO_3, MoO_2, WO_3, and WO_2 for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb.
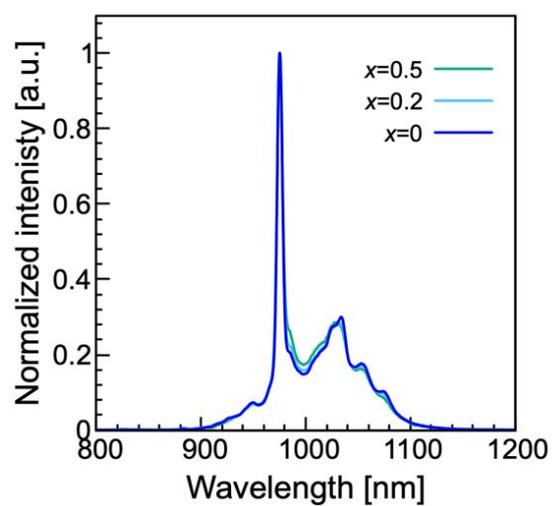
Figure S11. Normalized PL spectra under 363 nm excitation for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb (x=0, 0.2, and 0.5).

Figure S12. Photographs of PDMS/GMO:Bi,Yb film.

Table. S1. Molar ratios of RE/Bi/Yb for REMO:Bi,Yb (RE=Gd, Y, Lu) estimated from XPS.

	GMO:Bi,Yb	YMO:Bi,Yb	LuMO:Bi,Yb
Gd [mol%]	90.4	83.0	95.5
Bi [mol%]	7.92	7.38	3.18
Yb [mol%]	1.67	9.65	1.32

Table S2. Lattice parameters for REMO:Bi,Yb (RE=Gd, Y, and Lu) refined by Rietveld analysis.

	GMO:Bi,Yb	YMO:Bi,Yb	LuMO:Bi,Yb
a [Å]	16.523(3)	16.382(2)	16.288(1)
b [Å]	11.168(2)	11.009(1)	10.8779(8)
c [Å]	5.398(1)	5.334(6)	5.2658(6)
β [°]	108.460(9)	108.64(5)	108.805(9)
V [Å^3]	945.4(3)	911.5(2)	883.2(2)
R_{wp} [%]	2.98	5.223	7.616
R_p [%]	2.286	3.846	5.337
S	3.375	4.854	7.426
Impurity phase [%]	-	7.8	4.3

Table S3. Lattice parameters for REMO (RE=Gd, Y, and Lu) refined by Rietveld analysis.

	GMO	YMO	LuMO
a [Å]	16.572(8)	16.392(3)	16.318(6)
b [Å]	11.159(4)	11.017(2)	10.878(2)
c [Å]	5.405(2)	5.3372(9)	5.265(2)
β [°]	108.43(2)	108.603(7)	108.81(5)
V [Å^3]	948.6(7)	913.5(2)	884.3(5)
R_{wp} [%]	3.922	5.868	11.17
R_p [%]	2.639	4.280	7.791
S	4.839	5.453	10.741
Impurity phase [%]	1.2	5.0	15

Table S4. Fitting parameters of decay curves for REMO:Bi,Yb (RE=Gd, Y, and Lu).

Sample	τ_1 [μs]	τ_2 [μs]	A_1 [-]	A_1 [-]	τ_{ave} [μs]
GMO:Bi,Yb	97.3	265	583	410	207
YMO:Bi,Yb	62.6	160	708	303	113
LuMO:Bi,Yb	36.0	117	838	139	64.4

Table S5. Fitting parameters of decay curves for $Gd_2Mo_{1-x}W_xO_6$:Bi,Yb

x	τ_1 [μs]	τ_2 [μs]	A_1 [-]	A_1 [-]	τ_{ave} [μs]
0	97.3	265	583	410	207
0.2	101	275	650	381	208
0.5	77.4	257	650	381	213