Supporting Information

Unlocking Color-Tunable Emission of Eu^{2+}-Activated Phosphors through Doping-Free Exploration of Hidden Sites

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Supporting Figures:

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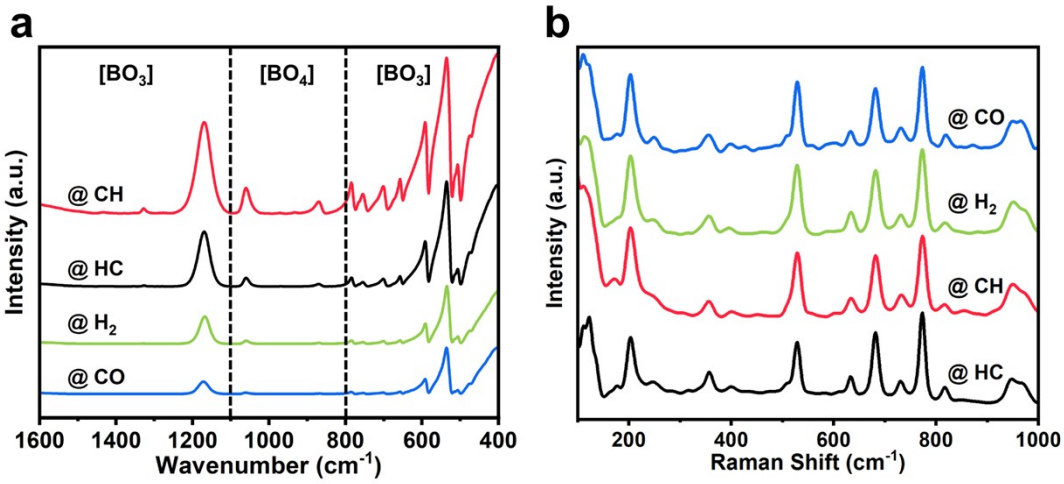

Fig. S1 (a) Fourier transform infrared (FT-IR) spectra and (b) Raman spectra of NBB:Eu^{2+}@CO, NBB:Eu^{2+}@H_2, NBB:Eu^{2+}@CH and NBB:Eu^{2+}@HC samples.

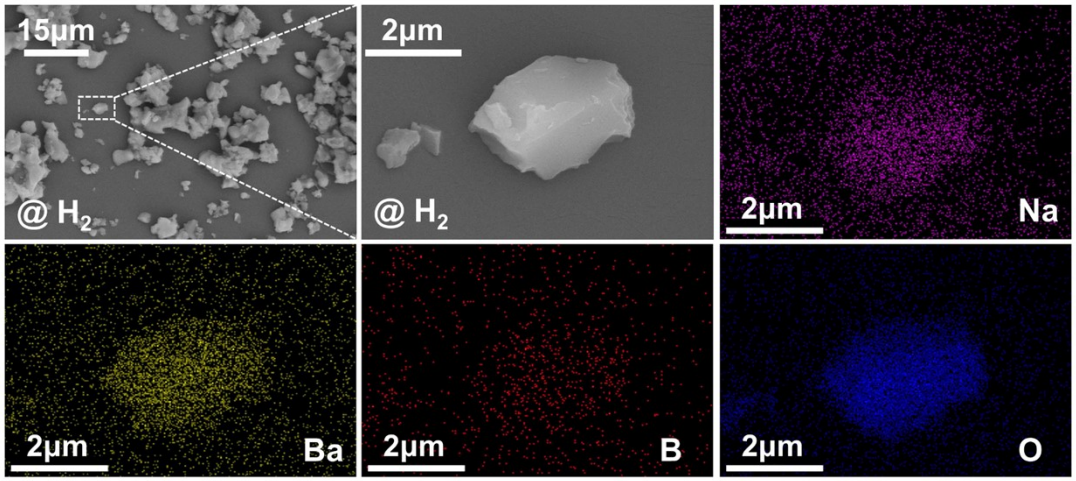

Fig. S2 SEM images and the corresponding elemental mapping images of NBB:Eu^{2+}@H_2 sample.

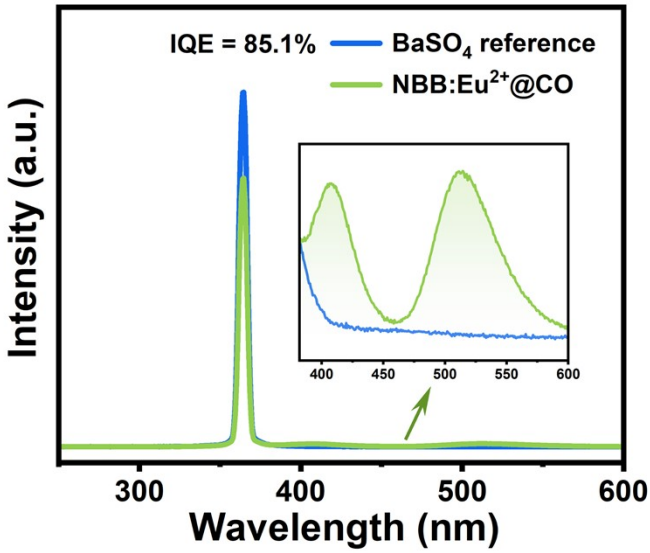

Fig. S3 IQE of NBB:0.03Eu^{2+}@CO sample.

The internal quantum efficiency (IQE) can be calculated by the following equation:

$$IQE = \frac{\int L_S}{\int E_R - \int E_S} \quad (1)$$

where $\int L_S$ represents the integral area of emission spectrum, $\int E_R$ and $\int E_S$ represent the integral area of excitation spectrum without and with the phosphor in the integrating sphere, respectively. As shown in the figure, under 365 nm excitation, the values of IQE of NBB:0.03Eu^{2+}@CO is calculated to be 85.1%.

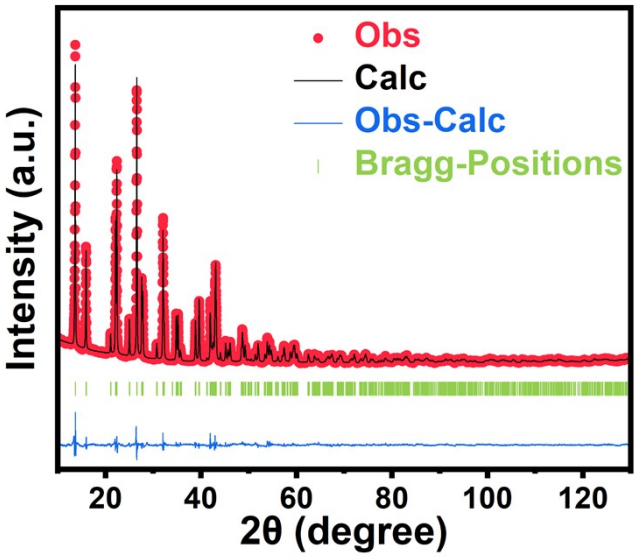

Fig. S4 Rietveld refinement of XRD patterns of NBB:0.1Eu^{2+}@CH sample.

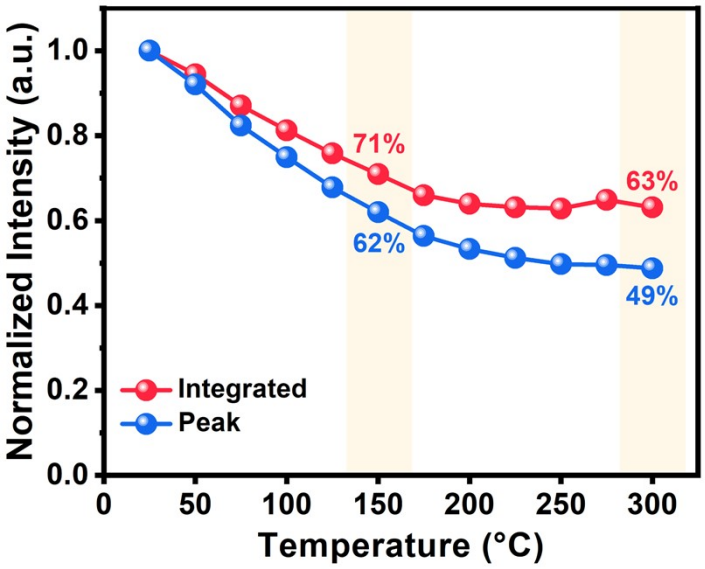

Fig. S5 Normalized integrated emission and peak intensity of NBB:0.03Eu^{2+}@H_2 sample as a function of temperature.

Supporting Tables:

Table S1 Crystallographic data for NBB:Eu^{2+}@CO, NBB:Eu^{2+}@H_2 and NBB:Eu^{2+}@CH samples.

Formula	**NBB:Eu^{2+}@CO**	**NBB:Eu^{2+}@H_2**	**NBB:Eu^{2+}@CH**
Space group	*R*3*c*	*R*3*c*	*R*3*c*
a (Å)	11.09019(3)	11.09235(4)	11.08931(3)
b (Å)	11.09019(3)	11.09235(4)	11.08931(3)
c (Å)	17.42435(11)	17.41842(12)	17.42104(10)
Volume ($Å^3$)	1855.945	1856.037	1855.294
α = β(°)	90	90	90
γ (°)	120	120	120
R_p (%)	4.2190	3.7302	3.5794
R_{wp} (%)	5.7504	4.8144	4.7914
R_B (%)	6.1603	6.3781	4.4847
S	3.3505	2.8976	2.8161

Table S2 The IQE and thermal stability at 150 °C of the reported related Eu^{2+}-activated phosphors.

Phosphor	IQE (%)	Thermal stability at 150 °C (%)	Ref.
$BaAl_4Sb_2O_{12}:Eu^{2+}$	96.7	94	1
$CaO:Eu^{2+}@C+GeO_2$	76	-	2
$Sr(Li_2Al_2O_2N_2):Eu^{2+}$	80	96	3
$RbLi(Li_3SiO_4)_2:Eu^{2+}$	80	103	4
$(Sr,Ba)Y_2O_4:Eu^{2+}$	-	90	5
$BaLi_2Al_2Si_2N_6:Eu^{2+}$	54.8	85.9	6
$Rb_3YSi_2O_7:Eu^{2+}$	32.6	81	7
$NBB:Eu^{2+}@CO$	85.1	106	This work

Table S3 Structural parameters of NBB:Eu^{2+}@CO, NBB:Eu^{2+}@H_2 and NBB:Eu^{2+}@CH samples.

Atom	x	y	z	B (Å^2)	Occ.
NBB:Eu^{2+}@CO					
Na	0	0	0.22273(11)	1.096(15)	0.9621(13)
Eu	0	0	0.22273(11)	1.096(15)	0.0379(13)
Ba	0	0	0	1.096(15)	0.9379(13)
Eu	0	0	0	1.096(15)	0.0621(13)
B1	0.3783(9)	0.2523(9)	0.0504(4)	0.82(3)	1
B2	0.4455(8)	0.3893(8)	0.1684(4)	0.82(3)	1
B3	0.2548(8)	0.3552(8)	0.1117(4)	0.82(3)	1
O1	0.4774(3)	0.3328(5)	0.11429(17)	0.82(3)	1
O2	0.2528(4)	0.2548(4)	0.0571(2)	0.82(3)	1
O3	0.1933(4)	0.4277(3)	0.06567(19)	0.82(3)	1
O4	0.3601(4)	0.4265(4)	0.1619(3)	0.82(3)	1
O5	0.1087(5)	0.2275(3)	0.16330(18)	0.82(3)	1
NBB:Eu^{2+}@H_2					
Na	0	0	0.22228(13)	0.798(16)	0.9955(14)
Eu	0	0	0.22228(13)	0.798(16)	0.0045(14)
Ba	0	0	0	0.798(16)	0.9045(14)
Eu	0	0	0	0.798(16)	0.0955(14)
B1	0.3765(9)	0.2551(8)	0.0668(4)	0.59(4)	1
B2	0.4665(8)	0.4174(8)	0.1806(5)	0.59(4)	1
B3	0.2419(9)	0.3342(11)	0.1024(4)	0.59(4)	1
O1	0.4851(4)	0.3312(5)	0.11439(17)	0.59(4)	1
O2	0.2579(4)	0.2439(4)	0.0601(2)	0.59(4)	1
O3	0.2110(6)	0.4278(3)	0.06758(17)	0.59(4)	1
O4	0.3397(6)	0.4147(4)	0.1667(4)	0.59(4)	1
O5	0.0900(4)	0.2380(3)	0.1614(2)	0.59(4)	1

NBB:Eu^{2+}@CH					
Na	0	0	0.22208(11)	0.917(13)	1
Eu	0	0	0.22208(11)	0.917(13)	0
Ba	0	0	0	0.917(13)	0.9
Eu	0	0	0	0.917(13)	0.1
B1	0.3923(7)	0.2472(7)	0.0659(3)	1.07(3)	1
B2	0.4626(7)	0.4027(7)	0.1717(4)	1.07(3)	1
B3	0.2222(6)	0.3299(9)	0.1135(3)	1.07(3)	1
O1	0.4773(3)	0.3160(4)	0.11844(18)	1.07(3)	1
O2	0.2493(3)	0.2320(4)	0.05574(18)	1.07(3)	1
O3	0.1958(4)	0.4301(3)	0.06796(19)	1.07(3)	1
O4	0.3467(4)	0.4119(3)	0.1615(3)	1.07(3)	1
O5	0.1103(5)	0.2338(2)	0.15810(18)	1.07(3)	1

References

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