Supporting information

Site occupancies, VUV-UV-vis photoluminescence and X-ray radioluminescence of Eu^{2+} doped $RbBaPO_4$

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Table S1. The final Refined Structural Parameters of $RbBaPO_4$[e] Host.

Atom	Wyckoff position	x	y	z	Occ.	B_{iso}
Ba	4c	0.494(1)	0.75	0.305(2)	1	0.76(1)
Rb	4c	0.158(2)	0.75	0.587(4)	1	0.95(9)
P	4c	0.267(3)	0.25	0.416(3)	1	1.00(0)
O1	8d	0.199(9)	0.25	0.561(7)	1	1.00(0)
O2	4c	0.465(2)	0.25	0.418(6)	1	1.78(6)
O3	4c	0.203(8)	0.029(3)	0.343(8)	1	1.00(8)

[e] Symmetry: orthorhombic; space group: *Pnma*; lattice parameters: a = 7.8178(8) Å, b

= 5.7386(4) Å, c = 10.0586(0) Å, V = 451.26(8) Å^3, Z = 4; reliability factors: R_{wp} = 5.66 %, R_p = 3.83 % and R_B = 4.76 %.

Table S2. Bond Lengths (Å) of Ba^{2+}-O^{2-} and Rb^{+}-O^{2-} in $RbBaPO_4$ Sample.

Bonds	Lengths (Å)	Bonds	Lengths (Å)
Ba-O1	2.741	Rb-O1 (x2)	2.899
Ba-O1	2.881	Rb-O1	3.176
Ba-O2	2.796	Rb-O2	2.945
Ba-O2 (x2)	3.096	Rb-O3(x2)	2.950
Ba-O3 (x2)	2.739	Rb-O3(x2)	3.069
Ba-O3 (x2)	2.805	Rb-O3(x2)	3.177
Average	2.855		3.031

Table S3. The Emissions of Eu^{2+} at Ba^{2+}/Sr^{2+} Sites of Isomorphic Host Compounds $KSrPO_4$ and $KBaPO_4$.

Phosphor	Emission peak of Eu^{2+} at Ba^{2+}/Sr^{2+} site (nm)	Reference in manuscript
$KBa_{0.995}Eu_{0.005}PO_4$	420	[26]
$KBa_{0.97}Eu_{0.03}PO_4$	417	[19]
$KSr_{0.999}Eu_{0.001}PO_4$	422	[20]
$KSr_{0.995}Eu_{0.005}PO_4$	424	[26]

Table S4. Fitting parameters for the Synchrotron radiation middle-far IR spectrum of $RbBa_{0.995}Eu_{0.005}PO_4$ via the complex dielectric function.

$\omega_{0,k}$ (cm^{-1})	$\omega_{p,k}$ (cm^{-1})	γ_k
100.85	158.23	22.215
122.77	123.1	12.374
140.03	133.87	17.172
154.13	180.01	16.897

177.73	120.62	14.828
207.28	33.081	10.631
426.25	252.15	132.48
523.55	195.2	72.724
553.82	130.53	15.666
700.68	180.94	130.59
885.17	305.86	181.71
1000.7	282.26	47.122
1031.8	112.08	30.298
2062.9	985.92	1808.8

Table S5. Fitting Parameters via Inokuti-Hirayama (I-H) model and Yokota-Tanimoto (Y-T) model for $RbBa_{1-x}Eu_xPO_4$ (x = 0.04 and 0.08) samples.

x (model)	n_a (m^{-3})	n_d (m^{-3})	C_{DA} (m^6/s)	D (m^2/s)	C_{DD} (m^6/s)	R_{adj}^2
0.04 (I-H)	3.55×10^{26}	-	3.08×10^{-48}	-	-	0.995
0.08 (I-H)	7.04×10^{26}	-	3.32×10^{-48}	-	-	0.995
0.04 (Y-T)	7.98×10^{25}	2.75×10^{26}	2.53×10^{-48}	1.07×10^{-23}	1.78×10^{-50}	0.996
0.08 (Y-T)	1.95×10^{26}	5.14×10^{26}	2.51×10^{-48}	3.06×10^{-23}	2.20×10^{-50}	0.995

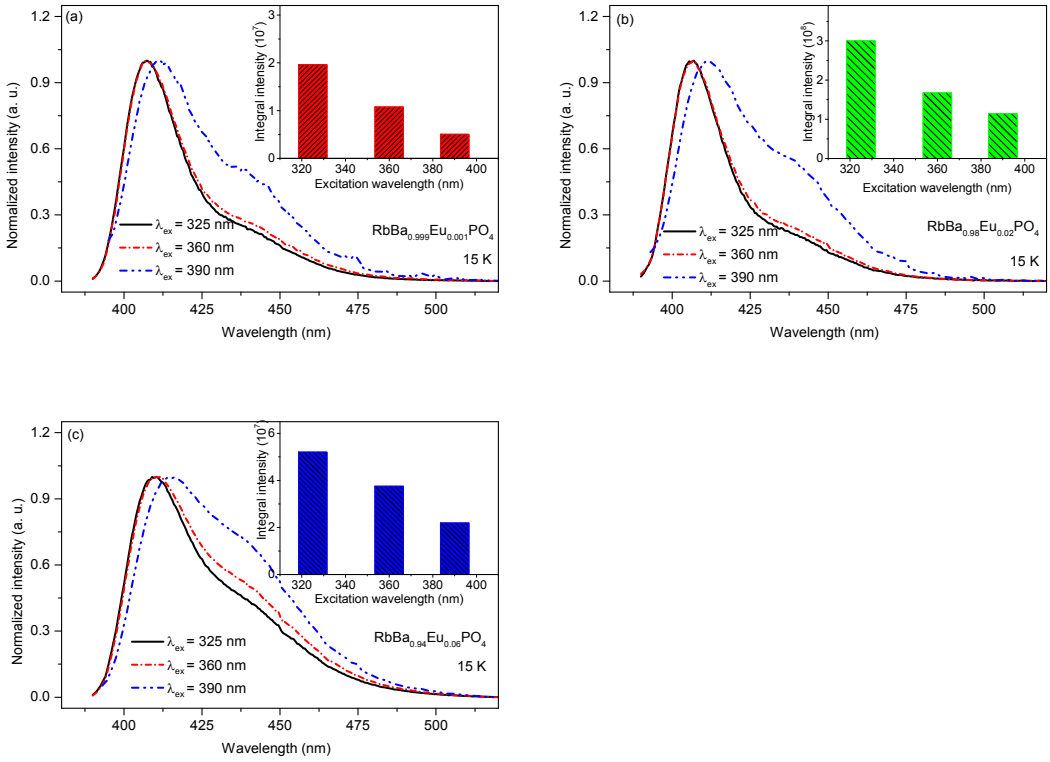


Figure S1. Highest-height normalized emission spectra of $RbBa_{1-x}Eu_xPO_4$ (a, x = 0.001; b, x = 0.02; c, x = 0.06, 15 K) under different excitation wavelengths; the insets in plots a, b and c are the excitation wavelength dependency of the total integral area, respectively, showing that the intensity of Eu^{2+} emission band decreases with the increase of excitation wavelength.

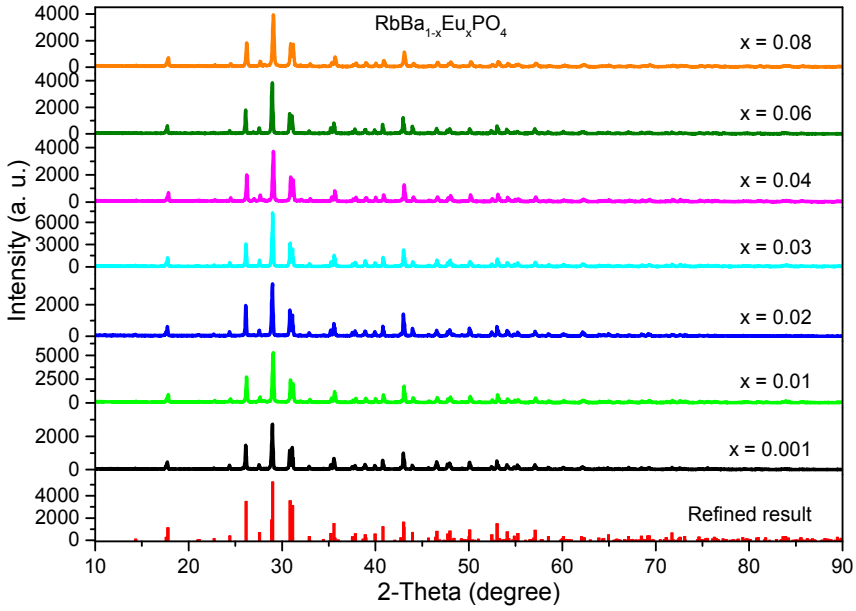


Figure S2. P-XRD patterns of $RbBa_{1-x}Eu_xPO_4$ (x = 0.001-0.08) samples and refined result of $RbBaPO_4$ host.

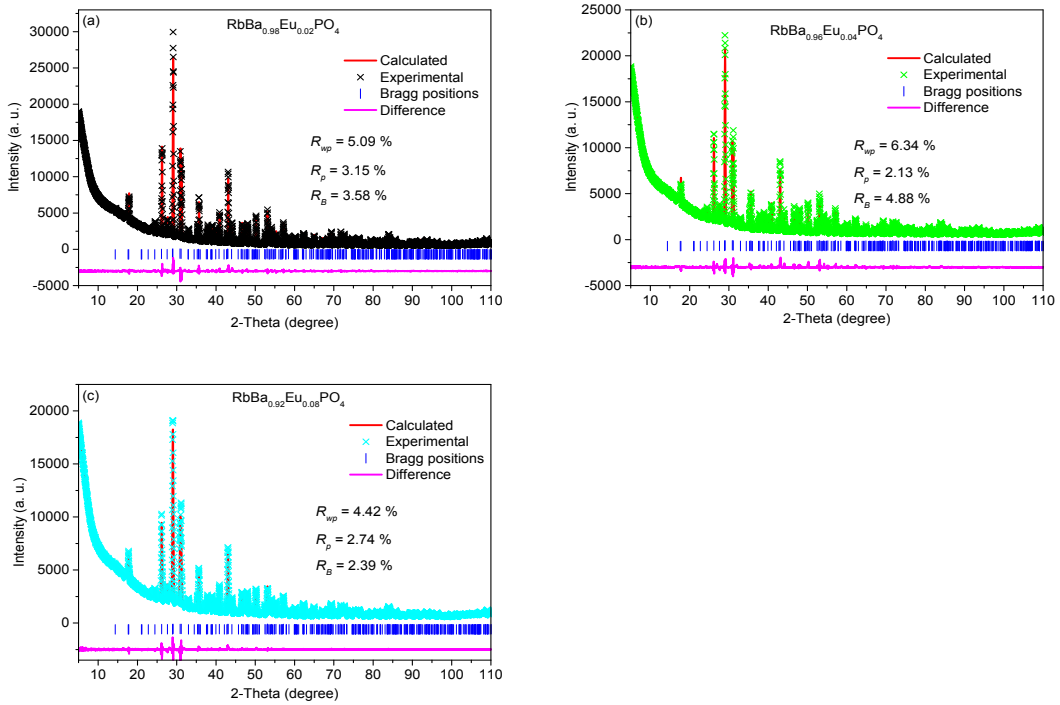


Figure S3. Rietveld refinement of P-XRD data of $RbBa_{1-x}Eu_xPO_4$ (a, x = 0.02; b, x = 0.04; c, x = 0.08) samples.

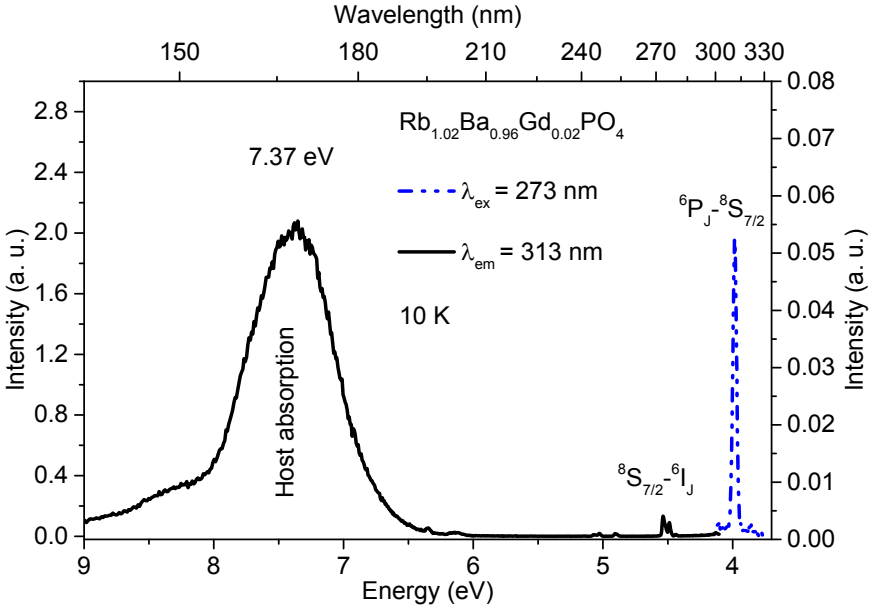
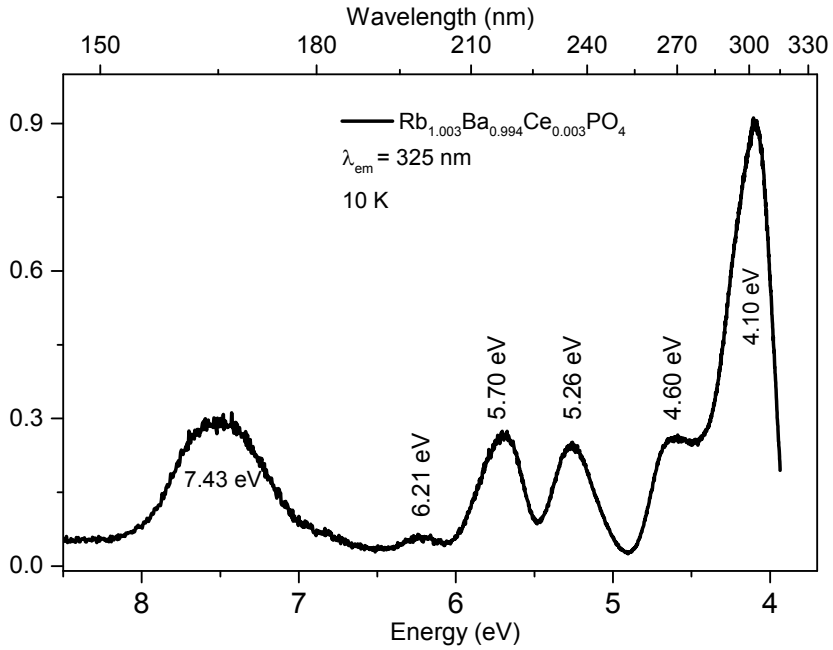


Figure S4. VUV-UV excitation (λ_{em} = 313 nm; 10 K) and emission (λ_{ex} = 273 nm; 10 K) spectra of $Rb_{1.02}Ba_{0.96}Gd_{0.02}PO_4$ sample.



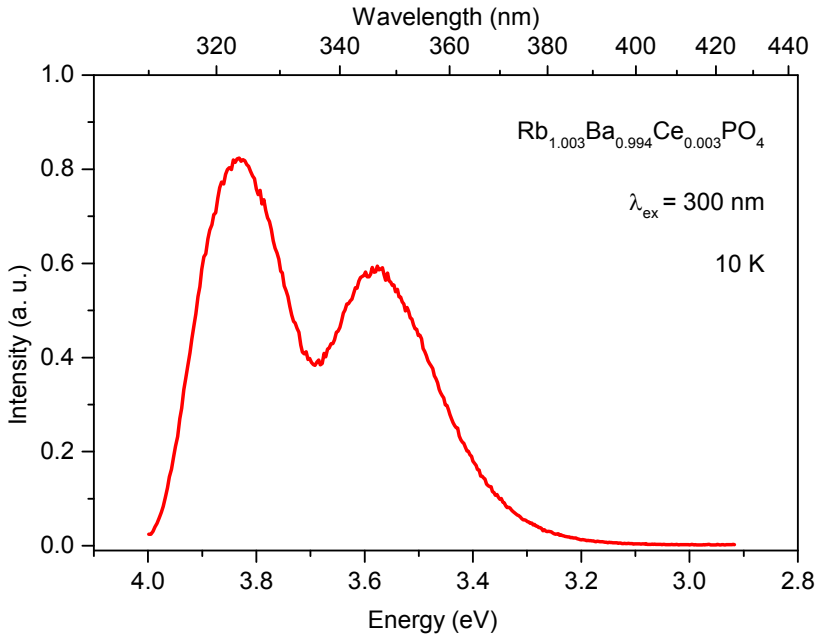


Figure S5. VUV-UV excitation (λ_{em} = 325 nm) and emission (λ_{ex} = 300 nm) spectra of $Rb_{1.003}Ba_{0.994}Ce_{0.003}PO_4$ sample at 10 K.

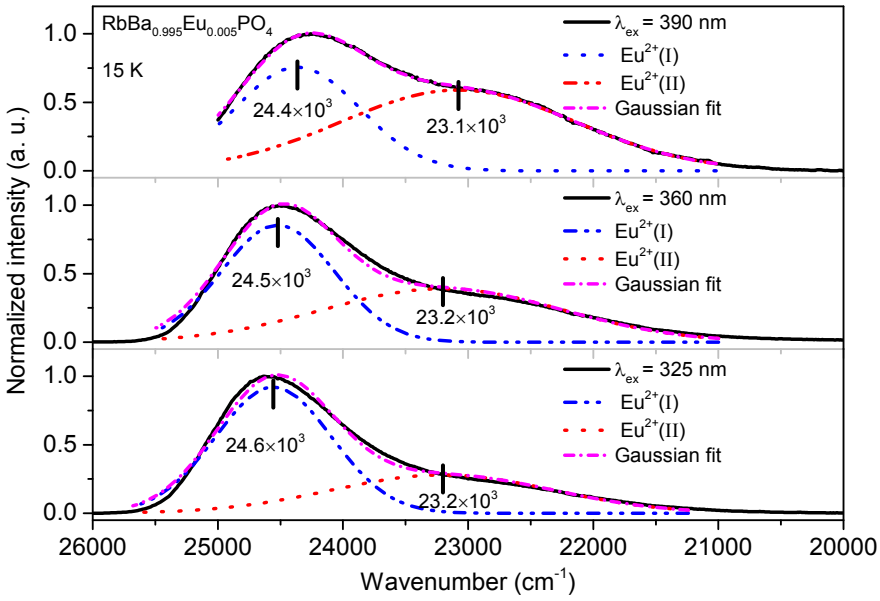


Figure S6. Highest-height normalized emission (λ_{ex} = 325, 360 and 390 nm; 15 K) spectra of $RbBa_{0.995}Eu_{0.005}PO_4$ sample and corresponding Gaussian fitting results.

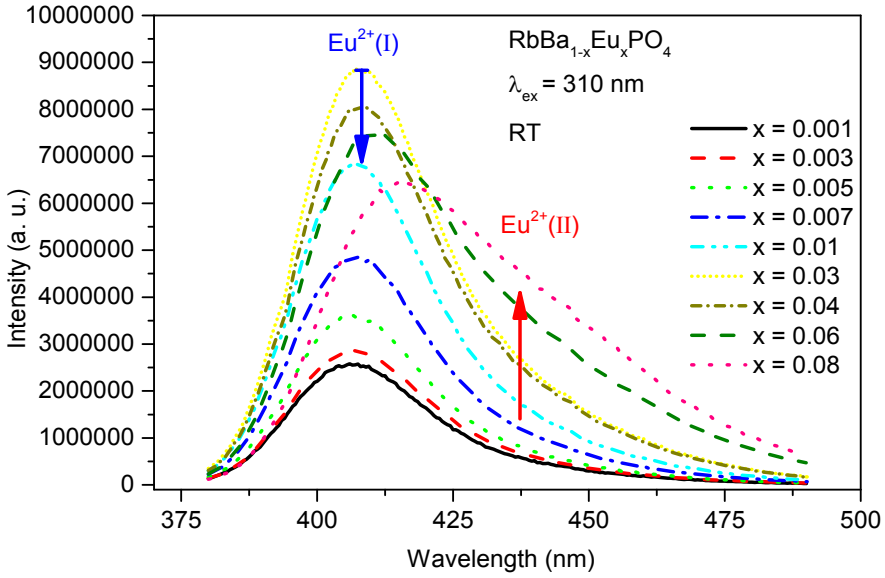


Figure S7. Emission spectra (λ_{ex} = 310; RT) of $RbBa_{1-x}Eu_xPO_4$ samples.