Supplementary Information

Structural Confinement Helps Achieve More Accurate Energy Transfer: Studies on the Garnet Structural NYGlG:Tb^{3+},Eu^{3+} Phosphors

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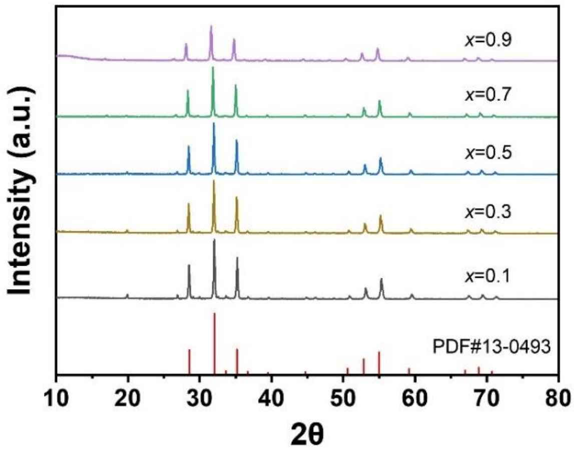

Fig. S1 XRD patterns of NYGIG: *x*Tb (*x*=0.1, 0.3, 0.5, 0.7, and 0.9).

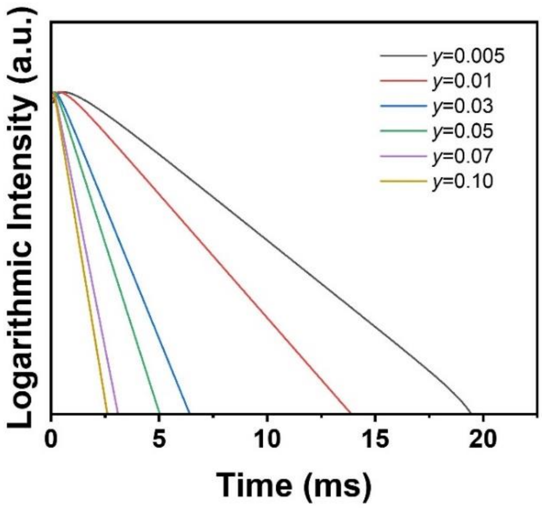

Fig. S2 The theoretical decay curves of Eu^{3+} in NYGIG: $0.5Tb^{3+}$, yEu^{3+} (y = 0.005-0.10).

Table S1 Crystal information and refinement parameters of NYGIG :$0.5Tb^{3+}$, $0.07Eu^{3+}$.

Phosphor	**NYGIG :$0.5Tb^{3+}$, $0.07Eu^{3+}$**
Crystal system	Cubic
Z	8
Space-group	$Ia\bar{3}d$
a=b=c	12.421 Å
V	1916.37 Å^3
GOF	2.52
R_p	8.96%
R_{wp}	13.21%

Table S2 XPS peak fit values for the synthesized $NaY_2Ga_2InGe_2O_{12}$.

Element	Peak labels	Peak Position (eV)	FWHM
Na	1s	1071.2	2.04
Y	$3d_{3/2}$, $3d_{5/2}$	159.4, 157.0	2.15, 1.74
Ga	3d①, 3d②	19.1,16.8	2.40, 2.40
In	$3d_{3/2}$, $3d_{5/2}$	450.7, 443.7	2.40, 1.54
Ge	3d	31.3	2.24
O	1s	530.4	2.57

Table S3 CIE chromaticity coordinates of NYGIG: $0.5Tb^{3+}$, yEu^{3+} phosphors.

y	**CIE *X***	**CIE *Y***
0.005	0.527	0.447
0.01	0.569	0.413
0.03	0.612	0.379
0.05	0.619	0.374
0.07	0.629	0.366
0.19	0.630	0.364

Table S4 Lifetime fittings for Tb^{3+} in NYGIG: $0.5Tb^{3+}$, yEu^{3+} phosphors

x	Measurement Mode	τ_1 (1st, ms)	R^2 (1st)
0	377 nm / 543 nm	2.02	0.9981
0.005	377 nm / 543 nm	1.01	0.9974
0.01	377 nm / 543 nm	0.61	0.9963
0.03	377 nm / 543 nm	0.25	0.9949
0.05	377 nm / 543 nm	0.20	0.9944
0.07	377 nm / 543 nm	0.12	0.9935
0.10	377 nm / 543 nm	0.10	0.9944

Table S5 The performance of NYGIG :$0.5Tb^{3+}$, $0.07Eu^{3+}$ phosphor in uv-excited LED with different operating current.

	Current (mA)	CIE	R_a	CCT(K)	Luminous efficiency (lm/W)
pc-WLEDs	20	0.3888, 0.3941	83.7	3909	0.59
	50	0.4031, 0.3818	83.4	3475	0.56
	100	(0.4024, 0.3801)	87.0	3476	0.49
	150	(0.4074, 0.380)	85.2	3363	0.44
	200	(0.4054, 0.377)	86.0	3382	0.40
	250	(0.4065, 0.3741)	85.8	3329	0.36
	300	(0.4079, 0.3748)	86.3	3304	0.33

Statistical Analysis: Impact of Na^+ Structural Confinement in $NaY_2Ga_2InGe_2O_{12}$

The crystal structure of $NaY_2Ga_2InGe_2O_{12}$: $0.5Tb^{3+}$, $0.07Eu^{3+}$ introduces Na^+ as a limiting ion, which significantly influences the spatial distribution and interactions of Tb^{3+} and Eu^{3+} ions.

Formation Probabilities with Na^+ Structural Confinement

1. Tb-Tb Pair Formation Probability: 25%
2. Eu-Eu Pair Formation Probability: 0.49%
3. Tb-Eu Pair Formation Probability: 7%

These probabilities suggest that the presence of Na^+ effectively reduces the likelihood of Tb^{3+} and Eu^{3+} ions clustering, thereby enhancing the energy transfer efficiency.

Formation Probabilities without Na^+ Structural Confinement

Assuming a random distribution of Y^{3+}, Tb^{3+}, and Eu^{3+} ions without Na^+ structural confinement:

1.**Y Occupancy**: $P(\mathrm{Y}) = \frac{2}{3} \times 0.93 = 0.62$

2.**Tb Occupancy**: $P(\mathrm{Tb}) = \frac{2}{3} \times 0.5 = 0.3333$

3.**Eu Occupancy**: $P(\mathrm{Eu}) = \frac{2}{3} \times 0.07 = 0.0467$

Tb-Eu Pair Formation Probability (considering both Tb-Eu and Eu-Tb pairs):

1. Tb followed by Eu:

$P(\mathrm{Tb\text{-}Eu}) = P(\mathrm{Tb}) \times \mathrm{P(Eu)} = 0.3333 \times 0.0467 = 0.0156 \approx 1.56\%$

2. Eu followed by Tb:

$P(\mathrm{Eu\text{-}Tb}) = \mathrm{P(Eu)} \times P(\mathrm{Tb}) = 0.0467 \times 0.3333 = 0.0156 \approx 1.56\%$

Total probability of forming a Tb-Eu pair:

$P(\mathrm{Eu\text{-}Tb})_{total} = 0.0156 + 0.0156 = 0.0312 \approx 3.12\%$

Formation of Tb-Tb Chains (2 to 6 Adjacent Tb Ions)

The probability of forming Tb-Tb chains of various lengths can be calculated as follows:

1. Tb-Tb Pair (2 adjacent Tb ions):

$P(\mathrm{Tb\text{-}Tb}) = P(\mathrm{Tb}) \times P(\mathrm{Tb} = 0.3333 \times 0.3333 = 0.1111 \approx 11.11\%$

2. Tb-Tb-Tb Chain (3 adjacent Tb ions):

$P(\mathrm{Tb\text{-}Tb\text{-}Tb}) = P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) = 0.3333 \times 0.3333 \times 0.3333 = 0.037 \approx 3.70\%$

3. Tb-Tb-Tb-Tb Chain (4 adjacent Tb ions):

$P(\mathrm{Tb\text{-}Tb\text{-}Tb\text{-}Tb}) = P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) = 0.3333 \times 0.3333 \times 0.3333 \times 0.3333 = 0.0123 \approx 1.23\%$

4. Tb-Tb-Tb-Tb-Tb Chain (5 adjacent Tb ions):

$P(\mathrm{Tb\text{-}Tb\text{-}Tb\text{-}Tb\text{-}Tb}) = P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) = 0.3333 \times 0.3333 \times 0.3333 \times 0.3333 \times 0.3333 = 0.0041 \approx 0.41\%$

5. Tb-Tb-Tb-Tb-Tb-Tb Chain (6 adjacent Tb ions):

$P(\mathrm{Tb\text{-}Tb\text{-}Tb\text{-}Tb\text{-}Tb\text{-}Tb}) = P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times \mathrm{P(Tb)} \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) \times P(\mathrm{Tb}) = 0.3333 \times 0.333 \times 0.3333 \times 0.3333 \times 0.3333 \times 0.3333 = 0.0014 \approx 0.14\%$

Total probability of forming Tb chains of any length:

$P(\mathrm{Tb\text{-}Tb}_{\text{chains of any length}}) = 11.11\% + 3.70\% + 1.23\% + 0.41\% + 0.14\% = 16.59\%$

Summary

In the absence of Na^+ structural confinement, the probability of forming a Tb-Eu pair is 3.12%, which is less than half of the probability under Na^+ confinement (7%). This indicates that without Na^+, the spatial distribution of Tb and Eu ions is less favorable for efficient energy transfer. Furthermore, without Na^+, it is easier for long Tb-Tb chains to form. For example, the overall probability of forming Tb chains of any length is 16.59%. This highlights the significant role of Na^+ in preventing the clustering of similar ions and improving energy transfer efficiency.