

Electronic Supplementary Information

Isotypic lanthanide-organic frameworks and scintillating films with colour-tunable X-ray radioluminescence for imaging applications

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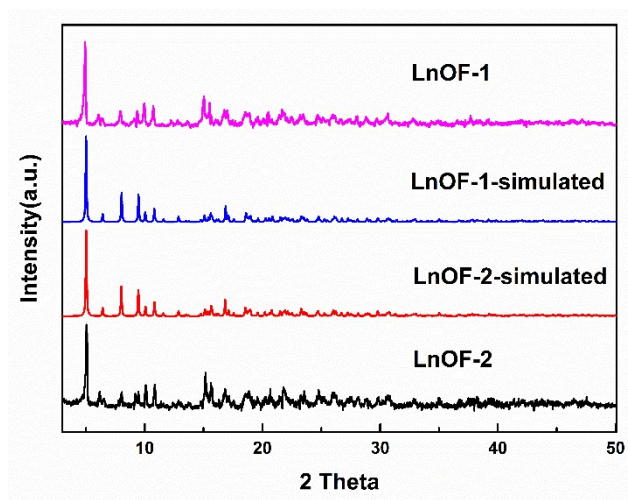


Fig. S1 The powdered X-ray diffraction (PXRD) patterns of LnOF-1 and LnOF-2.

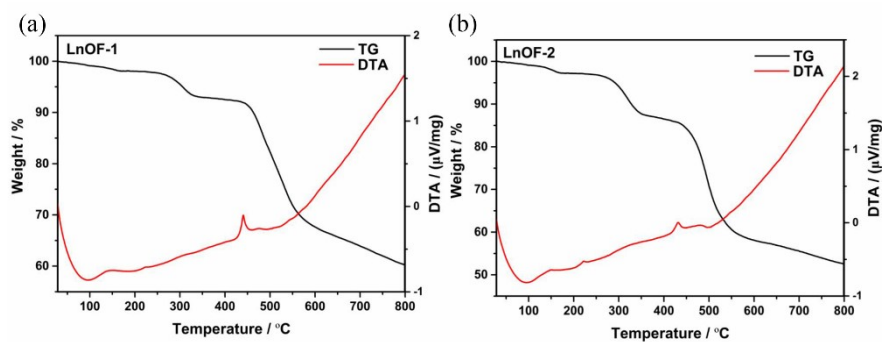


Fig. S2 The TG&DTA curves of (a) LnOF-1 and (b) LnOF-2.

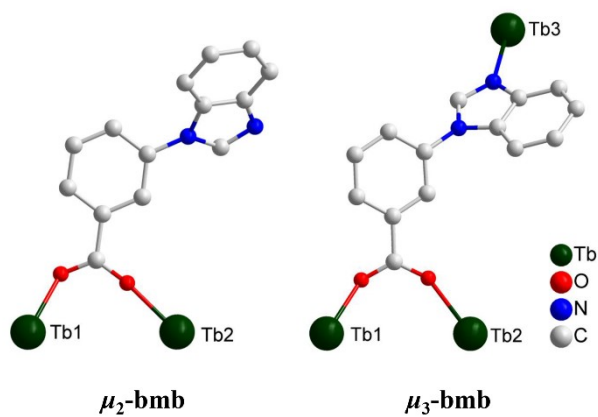


Fig. S3 The bridging modes of bmb⁻ ligand.

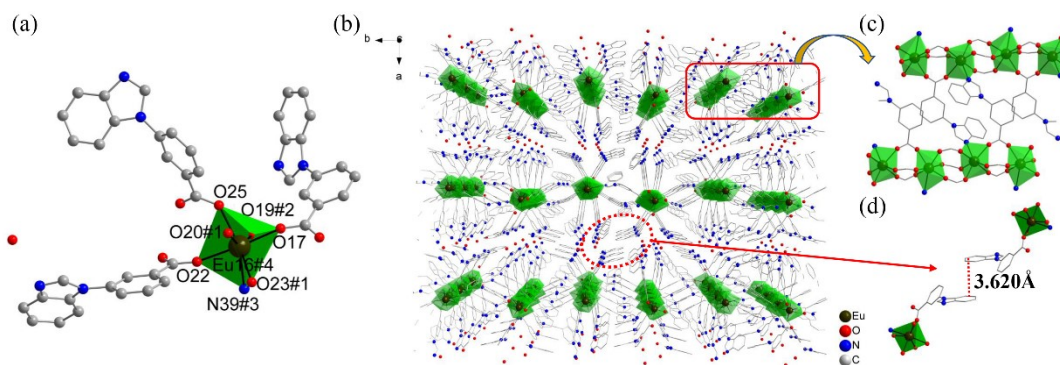


Fig. S4 (a) The asymmetric unit of LnOF-2. The symmetric codes for compound: #1 $x, 3/2 - y, 1/2 + z$; #2 $x, 1/2 - y, -1/2 + z$; #3 $1 - x, 1/2 + y, 1/2 - z$; #4 $1 - x, -1/2 + y, 1/2 - z$. (b) Illustration of the complete crystal structure of LnOF-2. (c) The coordination condition and connection mode of Eu^{3+} in the bc plane. (d) The distance between two benzimidazole groups from the adjacent layered structure is ca. 3.620 Å. Color code: Eu (olive green), O (red), N (blue), C (gray). For clarity, all hydrogen atoms are omitted.

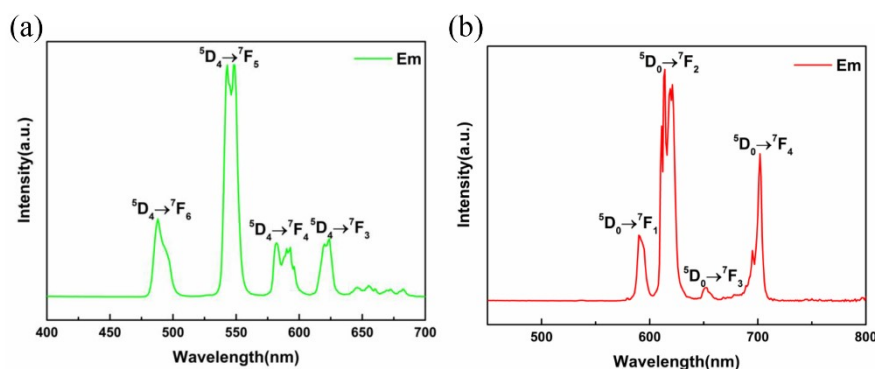


Fig. S5 The photoluminescence spectra of (a) LnOF-1 ($\lambda_{\text{ex}} = 314$ nm) and (b) LnOF-2 ($\lambda_{\text{ex}} = 312$ nm).

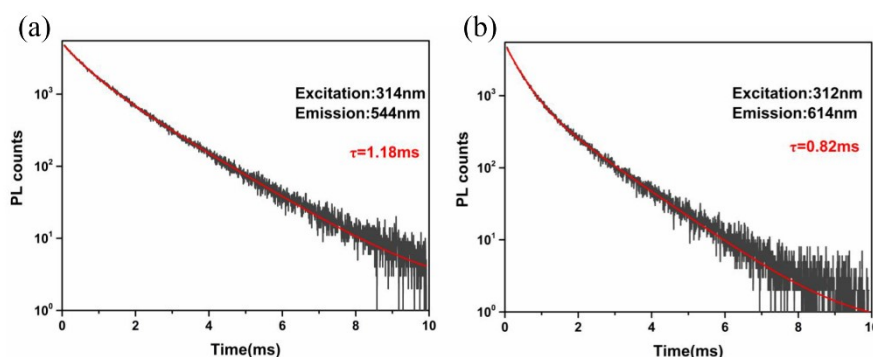


Fig. S6 The photoluminescence decay curves of (a) LnOF-1 and (b) LnOF-2.

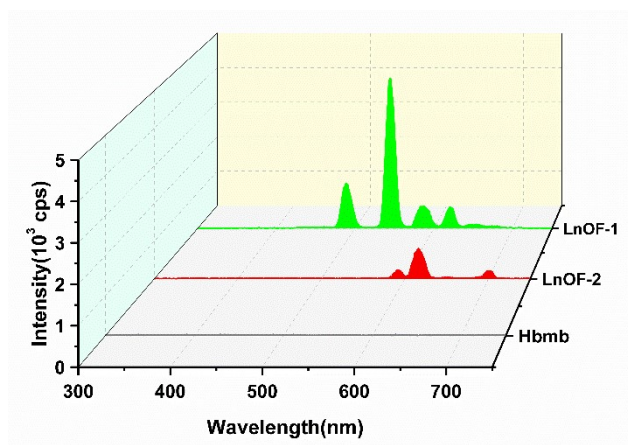


Fig. S7 The XEL spectra of Hbmb ligand, LnOF-1 and LnOF-2 with the X-ray tube voltage of 50 kV and the tube current of 100 μ A.

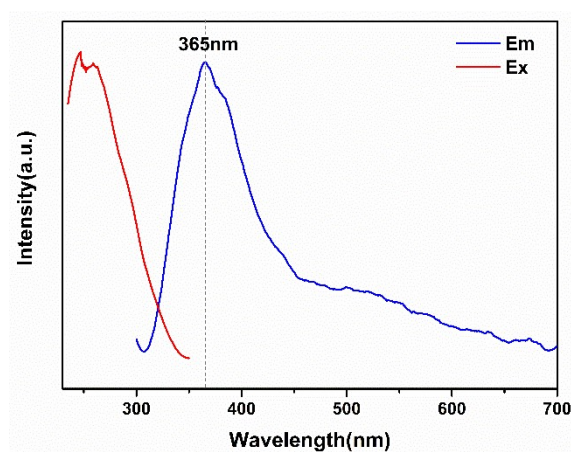


Fig. S8 The PL/PLE spectrum of Hbmb ligand.

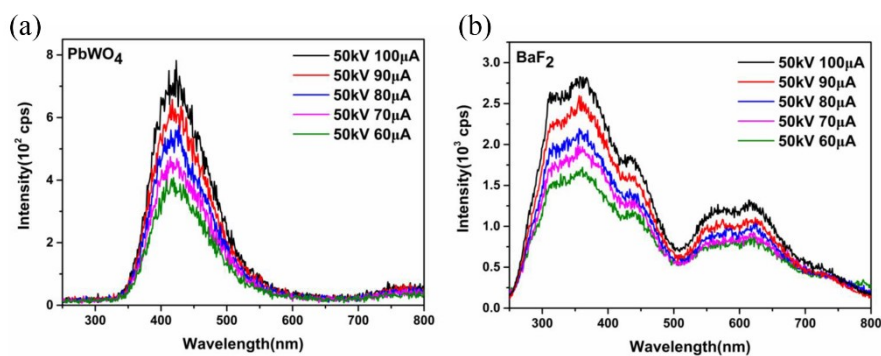


Fig. S9 The XEL spectra of powdered (a) PbWO_4 and (b) BaF_2 under exposure of X-ray tube with voltage fixed at 50 kV, current ranging from 60 to 100 μ A.

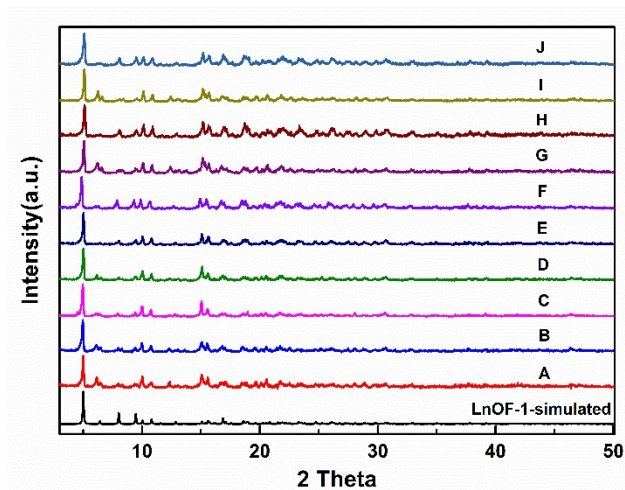


Fig. S10 The powdered X-ray diffraction (PXRD) patterns of $\text{Eu}_x\text{Tb}_{1-x}\text{-LnOFs}$. A~J represent that the doping ratios of Eu^{3+} and Tb^{3+} are 0.1% : 99.9%, 0.3% : 99.7%, 0.5% : 99.5%, 0.8% : 99.2%, 1% : 99%, 2% : 98%, 3% : 97%, 5% : 95%, 8% : 92% and 10% : 90%, respectively.

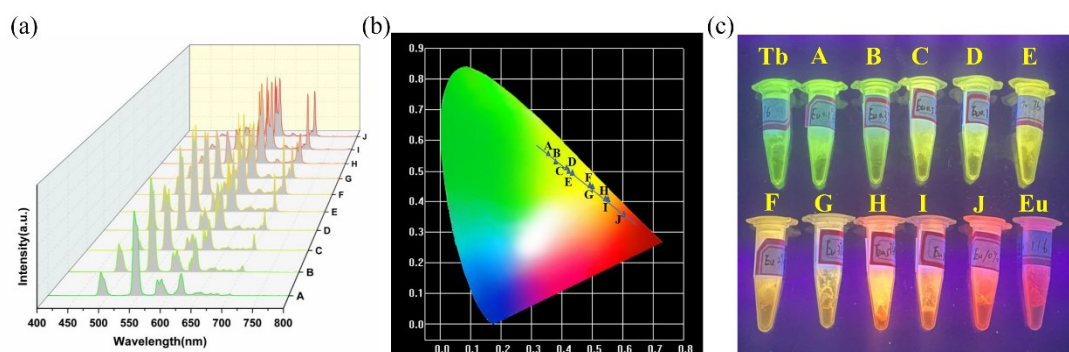


Fig. S11 (a) The photoluminescence spectra of $\text{Eu}_x\text{Tb}_{1-x}\text{-LnOFs}$ ($\lambda_{\text{ex}} = 312 \text{ nm}$). (b) Linear CIE chromaticity diagram of photoluminescence for $\text{Eu}_x\text{Tb}_{1-x}\text{-LnOFs}$. (c) The photograph of $\text{Eu}_x\text{Tb}_{1-x}\text{-LnOFs}$ under UV lamp.

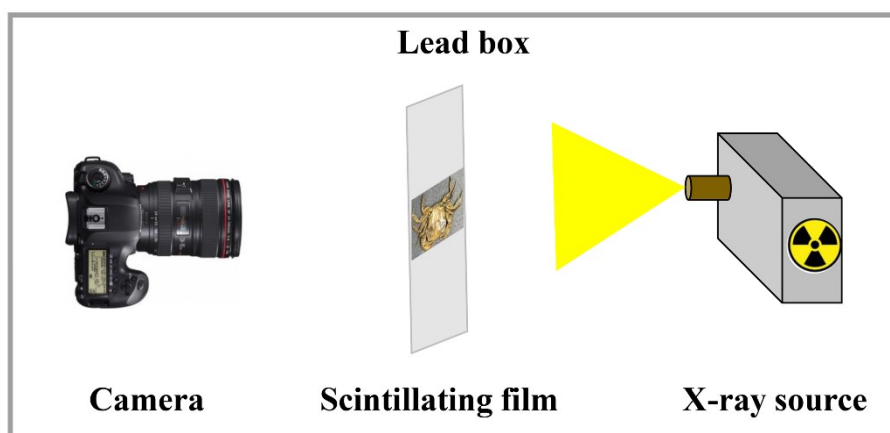


Fig. S12 Schematic diagram of the self-built X-ray imaging system.

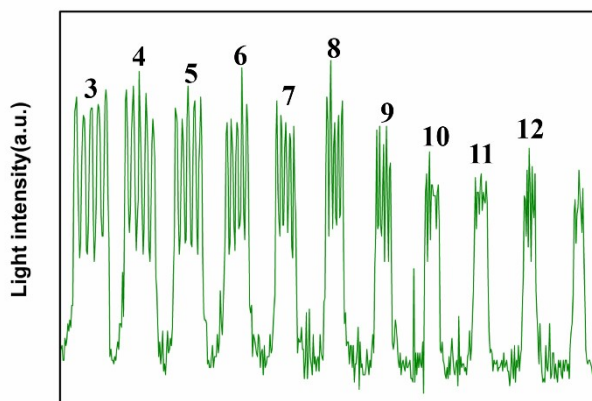


Fig. S13 The light intensity values corresponding to bright (I_{\max}) and dark (I_{\min}) stripes of each line pair.

Table S1 Crystallographic data for compounds.

Crystal data	LnOF-1	LnOF-2
CCDC number	2108315	2108316
Empirical formula	$C_{42}H_{29}N_6O_7Tb$	$C_{42}H_{29}N_6O_7Eu$
Formula weight	888.64	881.68
Temperature	293(2)	293(2)
Wavelength (\AA) / MoK_{α}	1.3405	1.3405
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a (\AA)	17.6637(2)	17.6275(11)
b (\AA)	22.0021(2)	22.066(1)
c (\AA)	9.5719(1)	9.6033(4)
α ($^{\circ}$)	90	90
β ($^{\circ}$)	94.459(1)	94.622(5)
γ ($^{\circ}$)	90	90
V (\AA^3)	3708.75(7)	3723.2(3)
Z	4	4
<i>Calcd.</i> density (g cm^{-3})	1.592	1.573
Absorption coefficient (mm^{-1})	10.221	9.114
)		
$F(000)$	1776	1768
Reflections collected	46785	47746
Completeness to $\theta = 53.54^{\circ}$	98.6%	98.6%
Data/restraints/parameters	8420/0/508	7387/3/512

Goodness-of-fit on F^2	1.015	1.071
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0303$	$R_1 = 0.0334$
	$wR_2 = 0.0759$	$wR_2 = 0.0883$

$${}^aR_1 = \sum(F_o - F_c)/\sum F_o, {}^b wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}.$$

Table S2 The Z_{eff} values (Tables S2†) of LnOF-1, LnOF-2 and some traditional inorganic scintillator materials.

Compounds	Z_{eff}
LnOF-1	42.27
LnOF-2	40.60
PbWO ₄	75.6
BaF ₂	52.7
Bi ₄ Ge ₃ O ₁₂	75.2

Empirical formulas (for a compound $A_xB_yC_z$):

$$Z_{\text{eff}} = [(xM_aZ_a^4 + yM_bZ_b^4 + zM_cZ_c^4)/(xM_a + yM_b + zM_c)]^{1/4}$$

where M_a , M_b and M_c are the atomic masses of A, B and C, respectively; Z_a , Z_b and Z_c are atomic numbers of A, B and C, respectively.

LnOF-1 (C₄₂H₂₉N₆O₇Tb):

$$Z_{\text{eff}} = [(42 \times 12.01 \times 6^4 + 29 \times 1.008 \times 1^4 + 6 \times 14.007 \times 7^4 + 7 \times 16.00 \times 8^4 + 1 \times 158.923 \times 65^4) / (42 \times 12.01 + 29 \times 1.008 + 6 \times 14.007 + 7 \times 16.00 + 1 \times 158.923)]^{1/4} = 42.27$$

LnOF-2 (C₄₂H₂₉N₆O₇Eu):

$$Z_{\text{eff}} = [(42 \times 12.01 \times 6^4 + 29 \times 1.008 \times 1^4 + 6 \times 14.007 \times 7^4 + 7 \times 16.00 \times 8^4 + 1 \times 151.964 \times 63^4) / (42 \times 12.01 + 29 \times 1.008 + 6 \times 14.007 + 7 \times 16.00 + 1 \times 151.964)]^{1/4} = 40.60$$