Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Multicolor and multimodal luminescence in Er^{3+} single-doped double perovskite for advanced anti-counterfeiting and encryption

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Computational Methods

The spin-polarized density functional theories were carried out by using the Vienna Ab initio Simulation Package (VASP). The Perdew-Burke-Ernzerhof generalized-gradient approximation functional was used to describe the interaction between electrons. The energy cutoff was set to 400 eV. The Monkhorst-Pack k-points grids were set to be 6×4×6 during the calculations. The vacuum region was set to be 15Å in the z direction to prevent the interaction between two adjacent surfaces. The energy convergence was set to 10^{-5} eV.

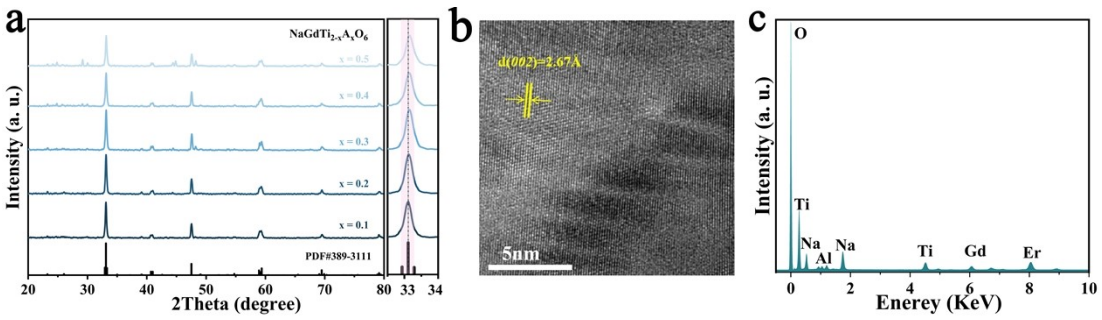

Figure S1. (a) XRD patterns with different Al^{3+} occupancy ratios of $NaGdTi_{2-x}Al_xO_6$ ($0.1 \leq x \leq 0.5$). (b) HRTEM image of NGTAO: Er^{3+}. (c)The EDS spectrum.

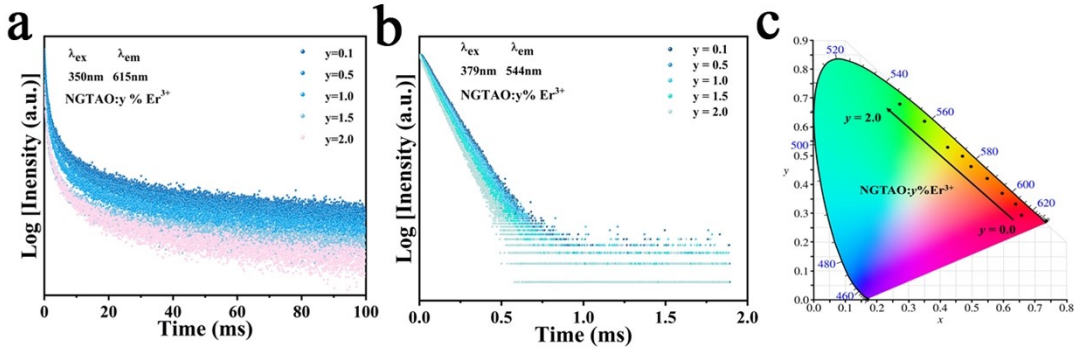

Figure S2. Luminescence decay curves of NGTAO: Er^{3+} samples measured at room temperature under 350 nm (a) and 379 nm (b) excitation. (c) CIE coordinates of the concentration-dependent color of NGTAO: y%Er^{3+} ($0.0 \leq y \leq 2.0$).

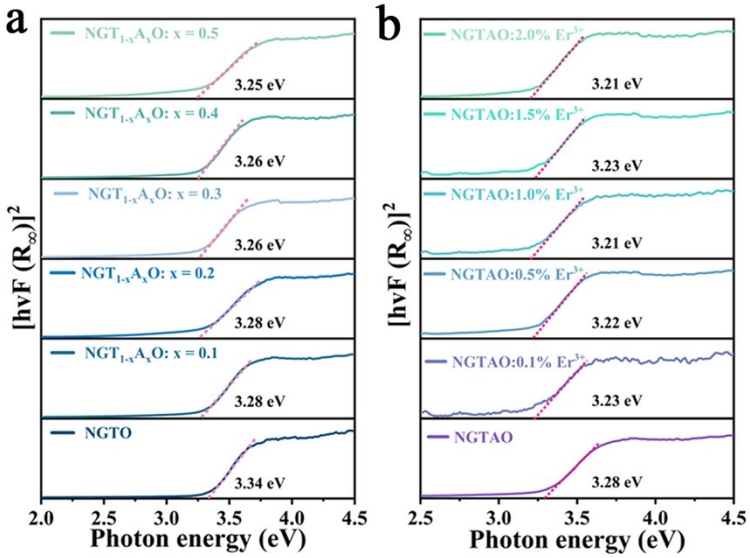

Figure S3. (a)The band gap values of NGTAO and (b)NGTAO: y%Er^{3+}.

Table S1. The refined crystallographic data of the NGTAO sample.

Formula	**NGTAO**
Space group name	*Pnma* (62)
a (Å)	5.435
b (Å)	7.646
c (Å)	5.379
α	90.000
β	90.000
γ	90.000
Unit-cell volume (Å^3)	223.534
T/K	297
Diffractometer	Rigaku D/Max-2400
Radiation/Å	Cu-Ka (λ= 1.5405)
Absorption correction	multi-scan
2θ range/°	20-80
R_{wp}	13.62%
R_p	9.66%
χ^2	0.69

Table S2. The fitting parameters of NGTAO: Er^{3+} decay curves.

Sample	τ_1	τ_2	τ_3	B_1	B_2	B_3	τ/ms
NGTAO	514.41	2816.09	18129.33	3252.90	1218.92	321.90	10.63
NGTAO:0.1%	2497.34	411.46	974.22	2503.44	274.13	19067.23	12.22
NGTAO:0.5%	3495.11	483.71	1159.16	2929.66	308.83	21789.99	13.32
NGTAO:1.0%	2970.34	472.42	1208.32	2851.97	367.1	20820.06	13.58
NGTAO:1.5%	1430.18	461.26	516.12	2884.80	154.01	21245.61	13.67
NGTAO:2.0%	1563.30	488.50	564.84	2921.30	160.88	22202.17	14.12

Table S3. The fitting parameters of NGTAO: Er^{3+} decay curves.

Sample	τ_1	B_1	τ/us
NGTAO:0.1%	95.05	5112.35	95.05
NGTAO:0.5%	93.63	4876.35	93.63
NGTAO:1.0%	90.09	4977.91	90.09
NGTAO:1.5%	82.14	4978.38	82.14
NGTAO:2.0%	75.96	4445.73	75.96