

Support information

Efficient broadband near-infrared emission induced by Nb⁵⁺ substitution for Ta⁵⁺

in GaTa_{1-y}Nb_yO₄: Cr³⁺ phosphor

*Lulu Lou^a, Shuang Zhao^a, Shuwen Yuan^a, Daoyun Zhu^c, Fugen Wu^{a, b, *}, Zhongfei Mu^{a,}*

*b, c, **

^a School of Materials and Energy, Guangdong University of Technology, Waihuan Xi Road, No.100, Guangzhou, 510006, PR China

^b Guangdong Provincial Key Laboratory of Information Photonics Technology, Guangdong University of Technology, Waihuan Xi Road, No.100, Guangzhou, 510006, PR China

^c Experimental Teaching Department, Guangdong University of Technology, Waihuan Xi Road, No.100, Guangzhou, 510006, PR China

Corresponding Authors

* E-mail: wufg@gdut.edu.cn.

* E-mail: muzhongfei@gdut.edu.cn.

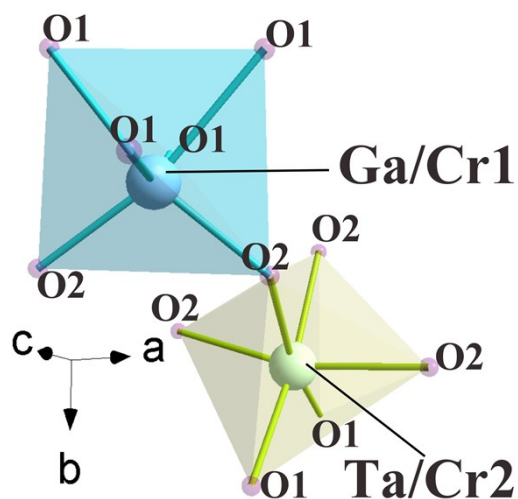


Figure S1. The microstructure of GTO.

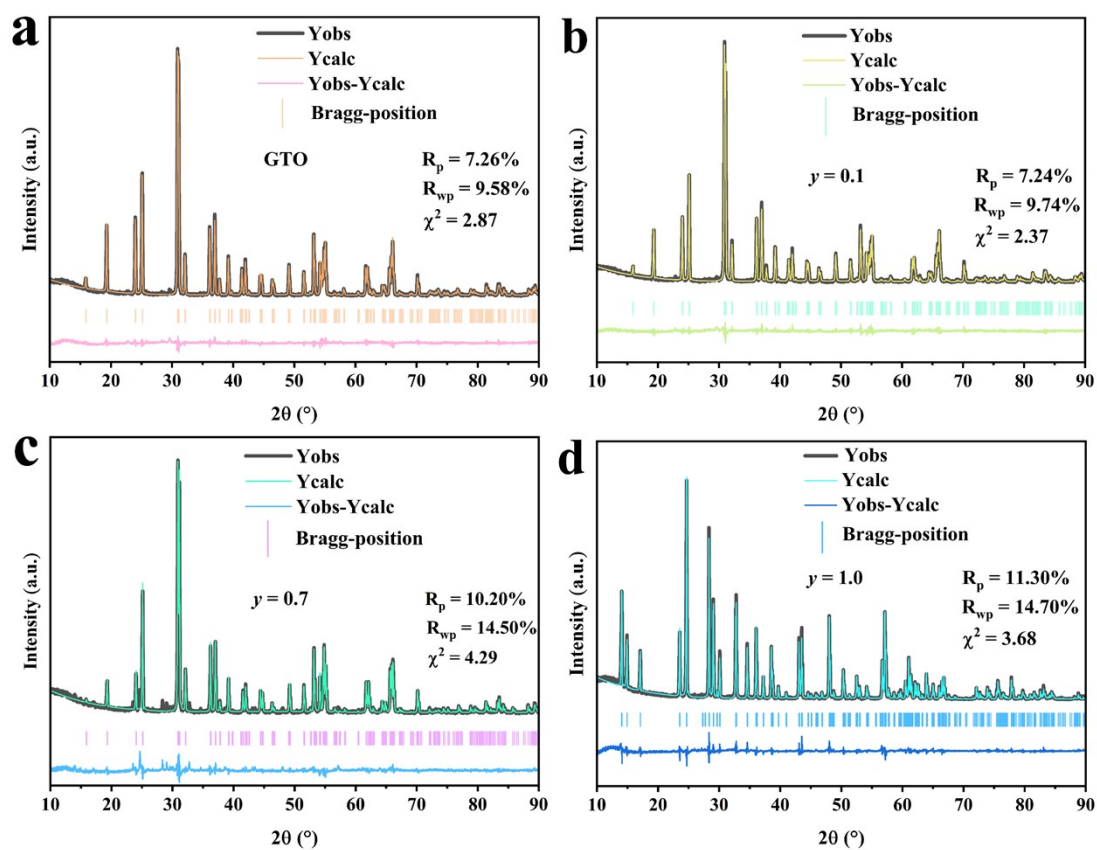


Figure S2. (a-d) Rietveld refinements of GTO and GTNO: 0.02Cr^{3+} ($y = 0.1, 0.7, 1.0$) samples.

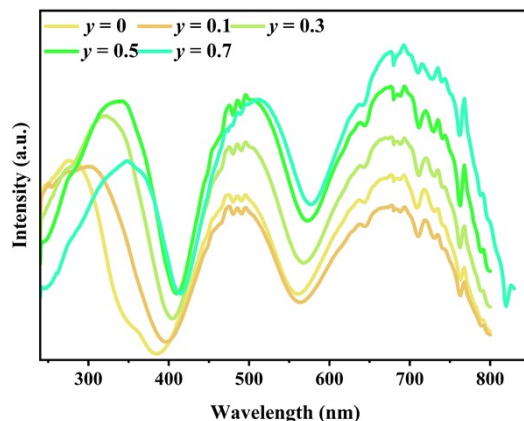


Figure S3. The PLE spectra of GTNO: 0.02Cr³⁺ ($y = 0-0.7$) phosphors monitored at 836, 839, 850, 865, 876 nm, respectively.

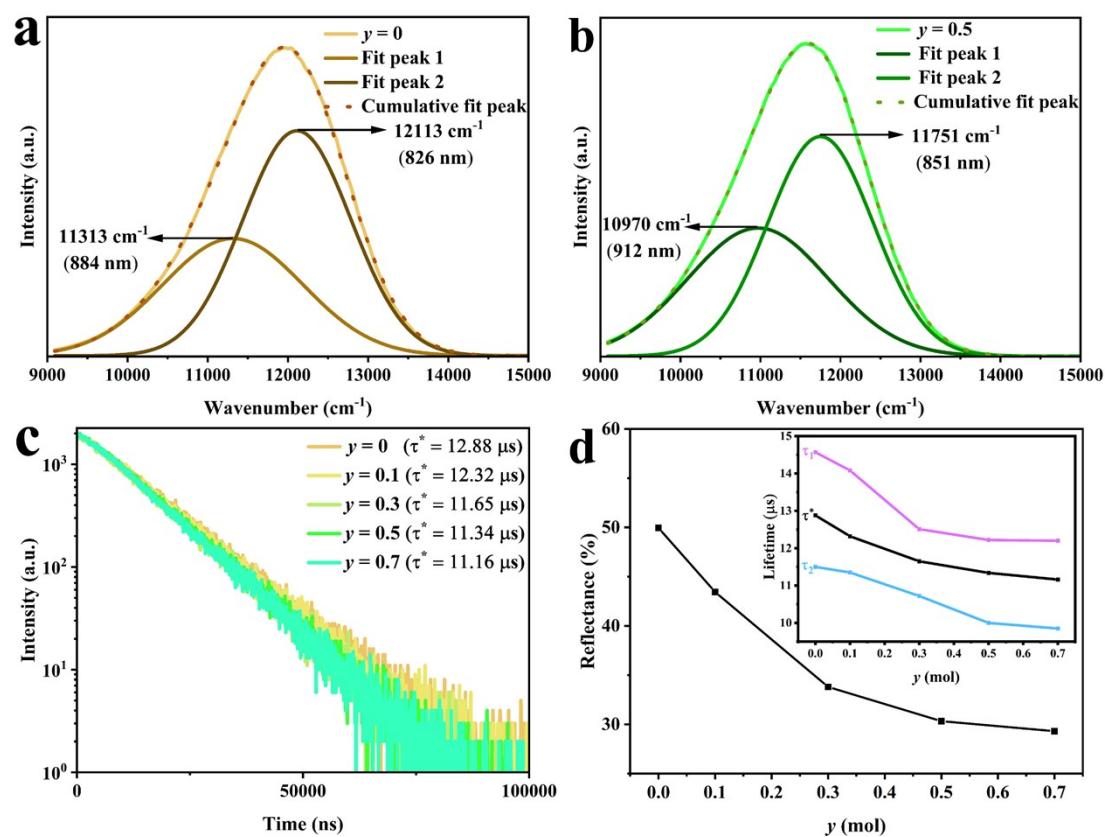


Figure S4. (a, b) Gaussian fitting and back-monitored for the PL and PLE spectra of the GTNO: 0.02Cr³⁺ ($y = 0, 0.5$) phosphors. (c) The PL decay curves of GTNO: 0.02Cr³⁺ ($y = 0-0.7$) phosphors monitored at 836, 839, 850, 865, 876 nm, respectively. (d) The reflectance and PL lifetime (in the inset) of GTNO: 0.02Cr³⁺ ($y = 0-0.7$) phosphors monitored at 474, 475, 476, 496, 501 nm, respectively.

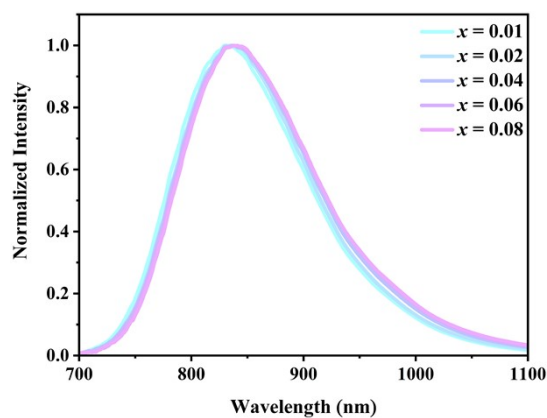


Figure S5. The PL spectra of GTO: $x\text{Cr}^{3+}$ ($x = 0.01-0.08$) phosphors monitored at 474 nm excitation.

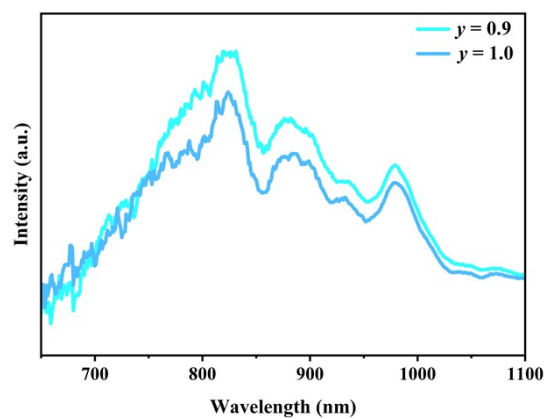


Figure S6. The PL spectra of GTNO: 0.02Cr^{3+} ($y = 0.9, 1.0$) phosphors.

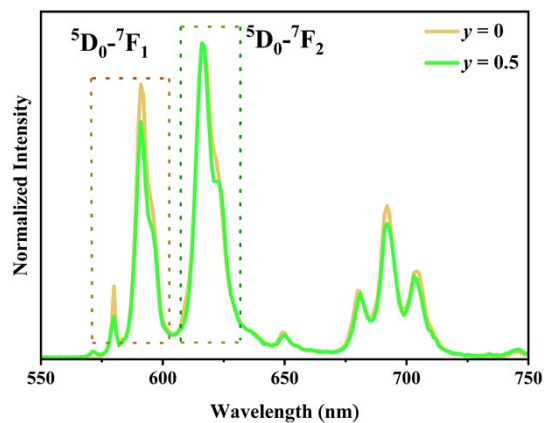


Figure S7. The PL spectra of GTNO: 0.02Eu^{3+} ($y = 0, 0.5$) phosphors.

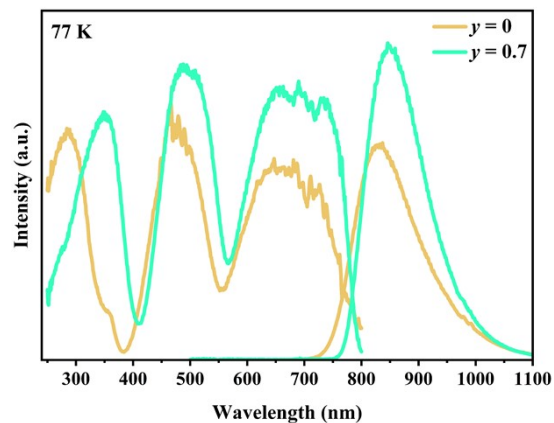


Figure S8. The PL and PLE spectra of GTNO: 0.02Cr³⁺ ($y = 0, 0.7$) phosphors at 77K.

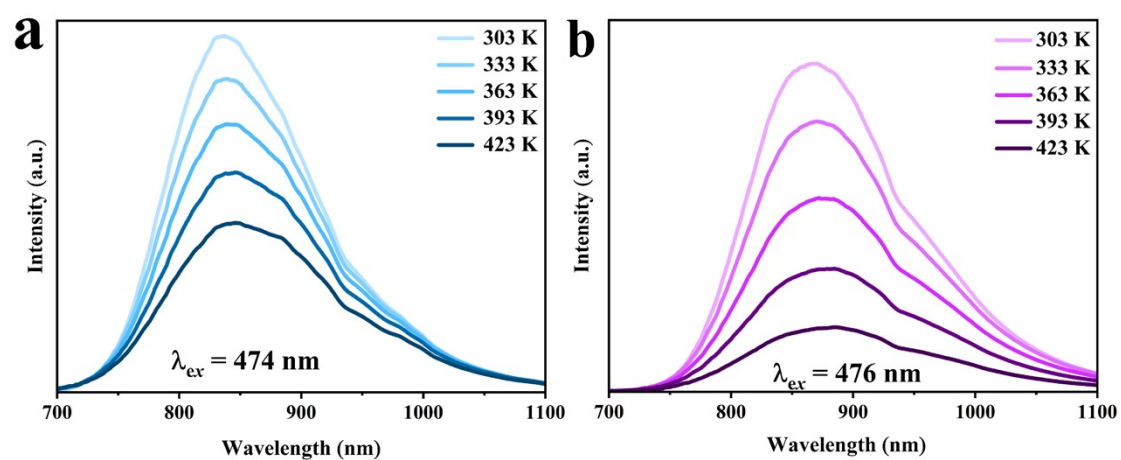


Figure S9. (a) Temperature-dependent spectra of GTNO: 0.02Cr³⁺ ($y = 0$) phosphor. (b) Temperature-dependent spectra of GTNO: 0.02Cr³⁺ ($y = 0.5$) phosphor.

Table S1The refined atomic positions of GTO and GTNO: 0.02Cr³⁺ ($y = 0, 0.5$) samples

GTO	Atom	Wyck. position	x	y	z	Occ.
	Ga	2f	0.5	0.6626(4)	0.25	0.5000
	Ta	2e	0	0.1797(5)	0.25	0.5000
	O1	4g	0.2103(3)	0.1230(8)	0.5823(9)	1.0000
	O2	4g	0.2749(1)	0.3881(2)	0.0796(2)	1.0000
GTNO: 0.02Cr³⁺ ($y = 0$)						
	Ga	2f	0.5	0.6596(9)	0.25	0.4933
	Ta	2e	0	0.1811(2)	0.25	0.4967
	O1	4g	0.2110(7)	0.1230(0)	0.5831(2)	1.0000
	O2	4g	0.2685(1)	0.3889(4)	0.0701(3)	1.0000
	Cr1	2f	0.5	0.6596(9)	0.25	0.0067
	Cr2	2e	0	0.1811(2)	0.25	0.0033
GTNO: 0.02Cr³⁺ ($y = 0.5$)						
	Ga	2f	0.5	0.6641(1)	0.25	0.4933
	Ta	2e	0	0.1816(4)	0.25	0.2467
	Nb	2e	0	0.1816(4)	0.25	0.2500
	O1	4g	0.2315(7)	0.1118(0)	0.5753(8)	1.0000
	O2	4g	0.2748(9)	0.3814(9)	0.0787(9)	1.0000
	Cr1	2f	0.5	0.6641(1)	0.25	0.0067
	Cr2	2e	0	0.1816(4)	0.25	0.0033

Table S2Refinement parameters of GTO and GTNO: 0.02Cr³⁺ ($y = 0, 0.1, 0.5, 0.7, 1.0$) samples

	a (Å)	b (Å)	c (Å)	V (Å³)	$\alpha = \gamma$ (°)	β (°)
GTO	4.5921 (6)	5.5689 (8)	4.9653 (0)	126.98	90	90.390
y = 0	4.5915 (8)	5.5677 (2)	4.9650 (6)	126.92	90	90.394
y = 0.1	4.5917 (1)	5.5669 (7)	4.9628 (0)	126.86	90	90.402
y = 0.5	4.5949 (8)	5.5685 (2)	4.9585 (4)	126.87	90	90.521
y = 0.7	4.5968 (4)	5.5692 (6)	4.9560 (7)	126.87	90	90.556
y = 1.0	12.4719 (9)	3.7866 (1)	6.6141 (8)	297.31	90	107.860

Table S3Main bond lengths (Å) of GTNO: 0.02Cr³⁺ ($y = 0, 0.1, 0.5, 0.7, 1.0$) samples

	$y = 0$	$y = 0.1$	$y = 0.5$	$y = 0.7$
Ga/Cr1-O1	1.974 (6)	1.934 (7)	1.952 (5)	1.903 (0)
Ga/Cr1 -O1	1.974 (6)	1.934 (7)	1.952 (5)	1.903 (0)
Ga/Cr1-O2	2.046 (1)	2.043 (6)	2.062 (9)	2.048 (2)
Ga/Cr1 -O2	2.046 (1)	2.043 (6)	2.062 (9)	2.048 (2)
Ga/Cr1 -O2	1.937 (1)	1.967 (0)	1.955 (2)	1.974 (5)
Ga/Cr1 -O2	1.937 (1)	1.967 (0)	1.955 (2)	1.974 (5)
Ta/Nb/Cr2 -O1	1.938 (4)	1.966 (6)	1.963 (4)	1.976 (2)
Ta/Nb/Cr2 -O1	1.938 (4)	1.966 (6)	1.963 (4)	1.976 (2)
Ta/Nb/Cr2 -O1	2.122 (2)	2.131 (3)	2.137 (4)	2.172 (8)
Ta/Nb/Cr2 -O1	2.122 (2)	2.131 (3)	2.137 (4)	2.172 (8)
Ta/Nb/Cr2 -O2	1.916 (1)	1.901 (2)	1.891 (5)	1.882 (8)
Ta/Nb/Cr2 -O2	1.916 (1)	1.901 (2)	1.891 (5)	1.882 (8)
		$y = 1.0$		
Ga/Cr1-O1		1.910 (5)		
Ga/Cr1-O2		1.878 (7)		
Ga/Cr1-O3		2.212 (1)		
Ga/Cr1-O4		2.044 (7)		
Ga/Cr1-O4		1.969 (8)		
Ga/Cr1-O4		1.969 (8)		
Ta/Nb/Cr2-O1		1.757 (3)		
Ta/Nb/Cr2-O2		1.898 (8)		
Ta/Nb/Cr2-O2		2.322 (2)		
Ta/Nb/Cr2-O3		1.934 (8)		
Ta/Nb/Cr2-O3		1.934 (8)		
Ta/Nb/Cr2-O4		2.228 (0)		

Table S4

Emission peak and FWHM of GTO: $x\text{Cr}^{3+}$ ($x = 0.01-0.08$) and GTNO: 0.02Cr^{3+} ($y = 0-0.7$) phosphors

GTO: $x\text{Cr}^{3+}$	Emission peak (nm)	FWHM (nm)
$x = 0.01$	830.41	136.91
$x = 0.02$	835.89	136.84
$x = 0.04$	836.89	140.11
$x = 0.06$	838.44	141.67
$x = 0.08$	840.44	140.03
GTNO: 0.02Cr^{3+}		
$y = 0$	835.89	136.84
$y = 0.1$	839.99	141.50
$y = 0.3$	851.03	145.51
$y = 0.5$	865.16	144.92
$y = 0.7$	876.20	149.14

Table S5

Crystal field strength (Dq/B) of GTNO: 0.02Cr^{3+} ($y = 0-0.7$) samples

	$y = 0$	$y = 0.1$	$y = 0.3$	$y = 0.5$	$y = 0.7$
Dq	1338	1334	1328	1300	1292
B (cm^{-1})	675.8	670.4	664.0	596.3	566.7
Dq/B	1.98	1.99	2.00	2.18	2.28

Table S6

The ratio of RT intensity and FWHM of GTNO: 0.02Cr^{3+} ($y = 0, 0.5$) phosphors

GTNO: 0.02Cr^{3+} ($y = 0$)	The ratio of RT intensity (%)	FWHM (nm)
303 K	100	137.91
333 K	90.94	141.82
363 K	80.70	145.49
393 K	68.60	149.08
423 K	54.91	154.15
GTNO: 0.02Cr^{3+} ($y = 0.5$)		
303 K	100	149.04
333 K	84.65	155.03
363 K	62.57	161.85
393 K	40.90	168.14
423 K	22.02	175.48

Table S7The NIR output power of NIR pc-LEDs fabricated by GTNO: 0.02Cr³⁺ ($y = 0, 0.5$) phosphors

Current (mA)	GTNO: 0.02Cr³⁺ ($y = 0$)		GTNO: 0.02Cr³⁺ ($y = 0.5$)	
	NIR output power (mW)	Full NIR output power (mW)	NIR output power (mW)	Full NIR output power (mW)
20	3.02	3.06	4.46	4.57
40	6.10	6.17	9.06	9.28
60	9.40	9.51	13.70	14.03
80	12.51	12.66	17.96	18.39
100	15.52	15.70	22.60	23.14
120	18.84	19.06	26.74	27.38
160	23.89	24.17	33.64	34.44
200	29.26	29.60	41.12	42.10
240	35.51	35.92	45.45	46.53
280	39.12	39.58	51.85	53.08
320	45.08	45.60	56.26	57.60

Table S8

The NIR photoelectric conversion efficiency of NIR pc-LEDs fabricated by GTNO: 0.02Cr³⁺ (y = 0, 0.5) phosphors

Current (mA)	GTNO: 0.02Cr ³⁺ (y = 0)		GTNO: 0.02Cr ³⁺ (y = 0.5)	
	Photoelectric conversion efficiency (%)	Full photoelectric conversion efficiency (%)	Photoelectric conversion efficiency (%)	Full photoelectric conversion efficiency (%)
20	6.16	6.23	9.10	9.32
40	6.04	6.11	8.97	9.18
60	6.14	6.21	8.95	9.16
80	5.98	6.05	8.59	8.79
100	5.83	5.90	8.49	8.69
120	5.80	5.87	8.25	8.45
160	5.42	5.48	7.63	7.81
200	5.19	5.25	7.32	7.49
240	5.08	5.14	6.61	6.77
280	4.76	4.82	6.35	6.50
320	4.69	4.74	5.92	6.06