

**Supporting Information for:**

**High-concentration Er<sup>3+</sup> ions singly doped GaTaO<sub>4</sub> single crystal for promising  
all-solid-state green laser and solid-state lighting applications**

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### 1. Figure S1.

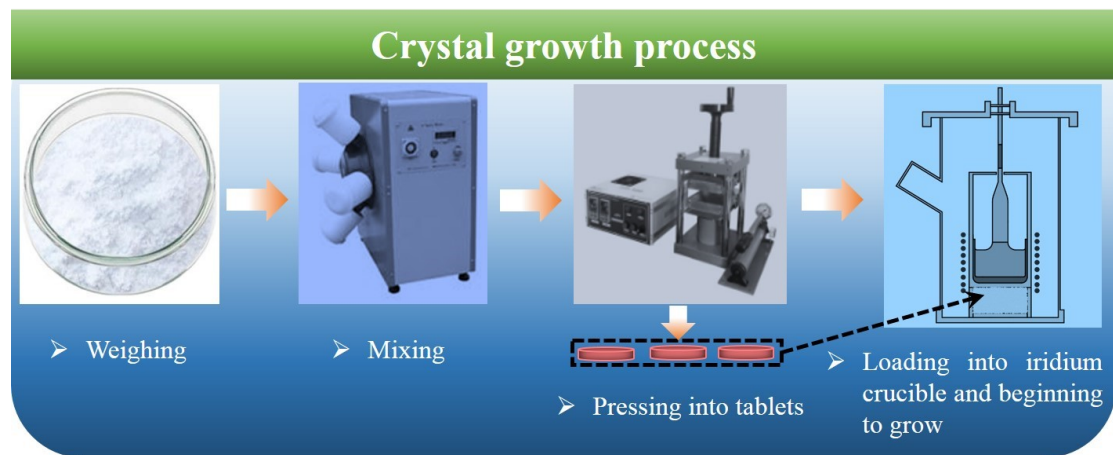


Figure S1. The schematic diagram of crystal growth process.

### 2. Figure S2

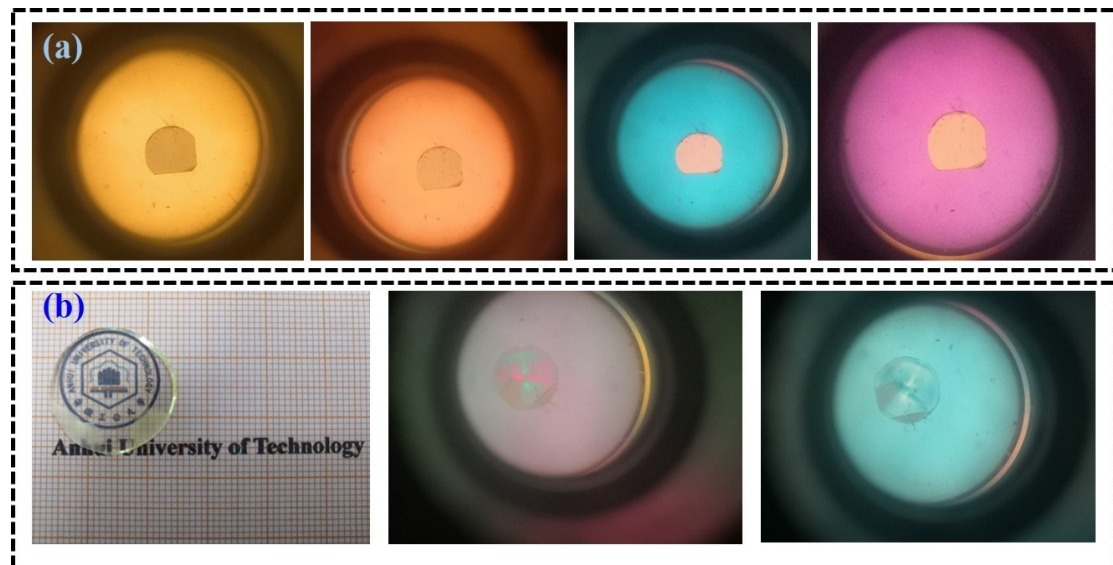


Figure S2. Residual thermal stress observation using a polarized stress meter. (a) No residual thermal stress observed in the as-grown Er:GdTaO<sub>4</sub> crystal; (b) The observed residual thermal stress in Dy:GSAG crystal (as a comparison).

### 3. Table S1

Table S1 The solved results for single-crystal X-ray diffraction

Structural formula	GdTaO <sub>4</sub>
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Space group	C2/c
Cell parameters	a=7.054 Å, b=11.041 Å, c=5.088 Å; $\alpha=\gamma=90^\circ$ , $\beta=130.35^\circ$
Z	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	57.66
F (000)	580.0
Maximum 2 $\theta$	54.94°
Total reflections	876
Unique reflections	359
R (int)	0.0972
R (sigma)	0.0875

#### 4. Table S2

Table S2 Comparison of the cell parameters for GdTaO<sub>4</sub> and Er:GdTaO<sub>4</sub>.

Sample	Cell parameters						Space group
	a (Å)	b (Å)	c (Å)	$\alpha=\gamma$	$\beta$	V (Å <sup>3</sup> )	
GdTaO <sub>4</sub> (ICSD#1 53362)[1]	7.054	11.078	5.082	90°	130.24°	303.15	C2/c (No.15)
Er:GdTaO <sub>4</sub>	7.054	11.041	5.088	90°	130.35°	302.00	C2/c (No.15)

#### 5. Figure S3

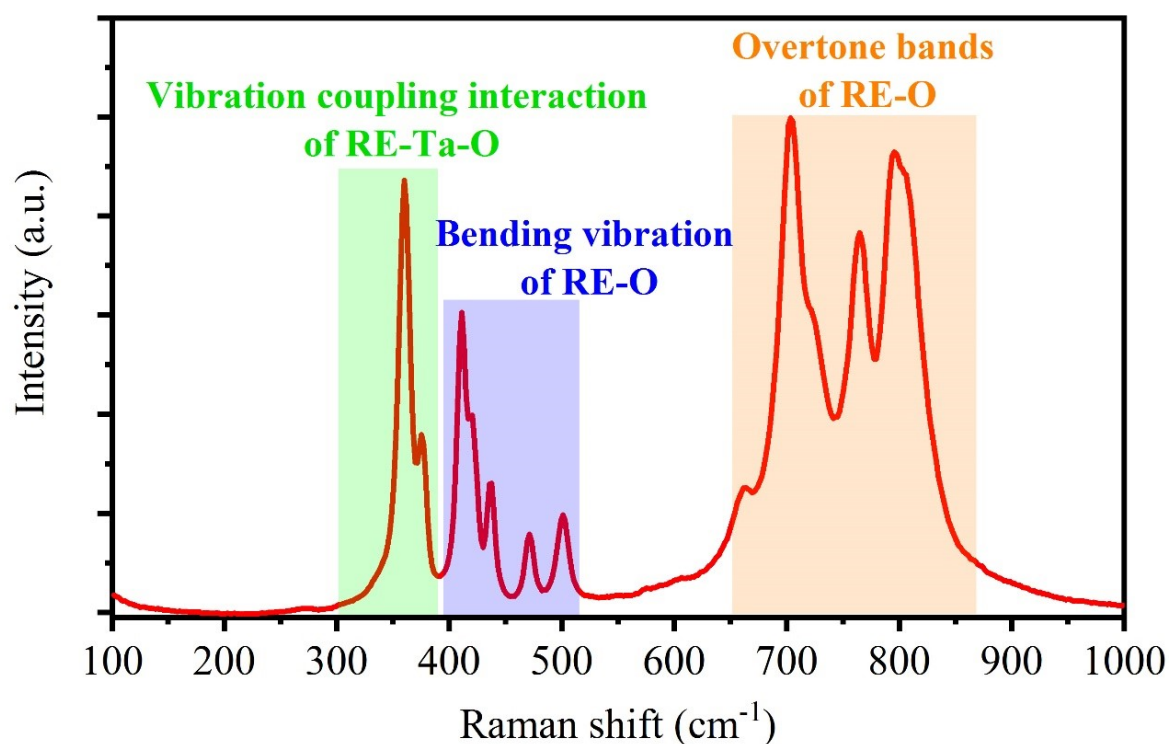


Figure S3. Room-temperature Raman spectrum of Er:GdTaO<sub>4</sub> crystal.

## 6. Figure S4



Figure S4. Crystal sample free from cleavage crack and cleavage crack along (010) face.

## 7. Effective segregation coefficient (Figure S5)

A crystal slice was cut from the should part of the as-grown Er:GdTaO<sub>4</sub> crystal and ground carefully into powder to determine the effective segregation coefficient of Er<sup>3+</sup> in GdTaO<sub>4</sub> host. A JSM—6490LV scanning electron microscopy (SEM) equipped with energy dispersive spectroscopy (EDS) was employed to determine the elements content. The measured mapping of the elements in Er:GdTaO<sub>4</sub> crystal is shown in Figure S5. The concentration of Er<sup>3+</sup> was estimated to be 11.0 at%, corresponding to an effective segregation coefficient ( $K_{eff}$ ) of 1.1, which is comparable to that reported in the Ref.[2] (0.95 for Er<sup>3+</sup> in 1 at.% Er:GdTaO<sub>4</sub> crystal). Therefore, the concentration of Er<sup>3+</sup> ( $N_C$ ) in GdTaO<sub>4</sub> host was calculated to be  $\sim 1.45 \times 10^{21} \text{ cm}^{-3}$ , according to the following equation:

$$N_C = \frac{10 \text{ at.\%} \times K_{eff} \times N_A \times \rho}{M} = \frac{0.1 \times 1.1 \times 6.02 \times 10^{23} \times 8.8}{403} / \text{cm}^3 = 1.45 \times 10^{21} / \text{cm}^3$$

Where  $N_A$  is the Avogadro's number,  $M$  is the molar mass,  $\rho$  is the density of the crystal, which was measured to be 8.8 g/cm<sup>3</sup> with the Archimedes principle method as shown in Figure S6.

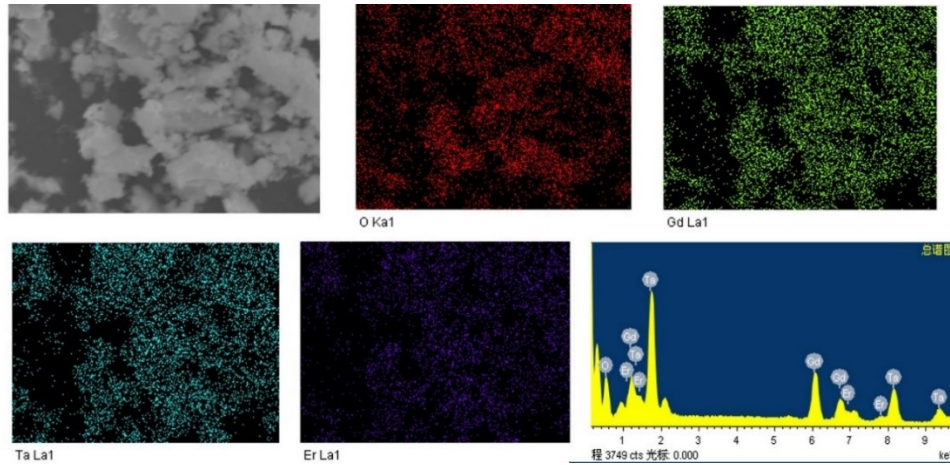


Figure S5. The mapping of the elements in Er:GdTaO<sub>4</sub> crystal.

### 8. Density measurement (Figure S6)

The density of the crystal was determined to be 8.8 g/cm<sup>3</sup> with the Archimedes principle method. Deionized water at room temperature was employed as the immersion liquid. The measurement was repeated five times and an average was taken to ensure the accuracy. The schematic diagram for the density measurement is shown in Figure S6.

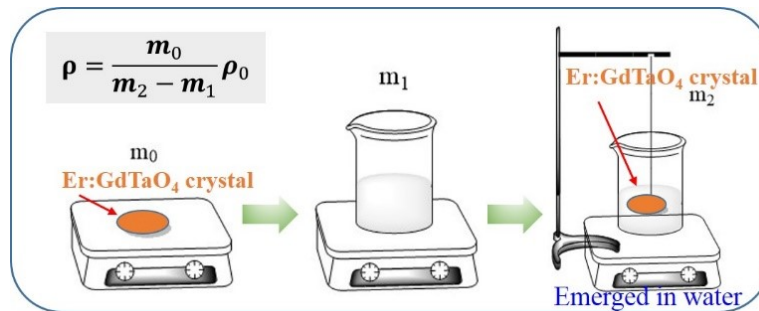


Figure S6. The schematic diagram for density measurement.

### 9. Figure S7

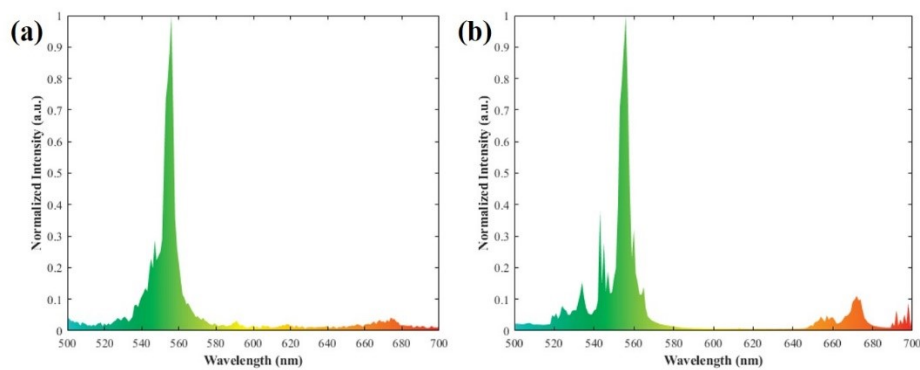


Figure S7. Emission spectra with color filled under the excitation of 450 nm(a) and 377 nm

(b).

## 10. Figure S8

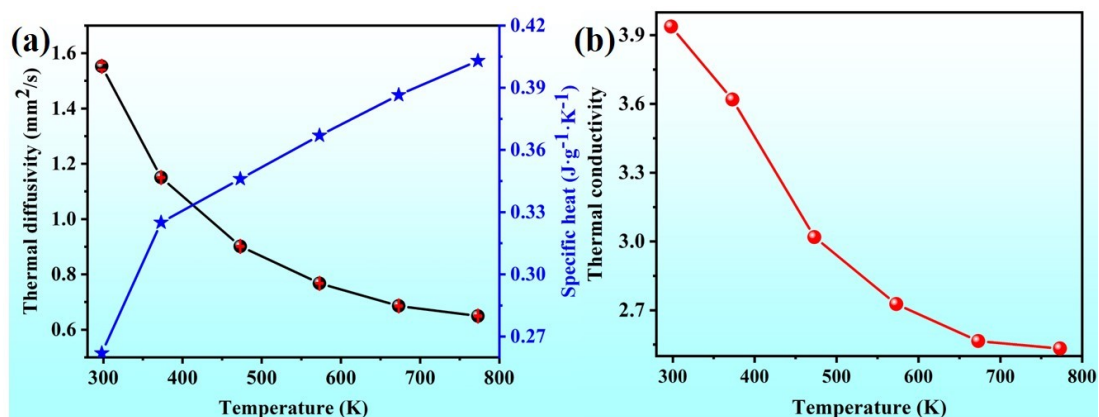


Figure S8. The specific heat, thermal diffusion coefficient (a) and thermal conductivity (b) of the crystal.

## 11. References

- [1] Tyitov, Y.O.; Bjelyavyina, N.; Slobodyanik, M.; Timoshenko, M. Peculiarities of the synthesis and polymorphic transformations and the crystalline structure of M-modifications of  $\text{LnTaO}_4$ . *Dopovydyi Natsyional'noyi Akademyiyi Nauk Ukrayini* **2004**, 145-50.
- [2] Chen, Y.; Peng, F.; Zhang, Q.; Liu, W.; Dou, R.; Ding, S.; Luo, J.; Sun, D.; Sun, G.; Wang, X. Growth, structure and spectroscopic properties of 1 at.%  $\text{Er}^{3+}:\text{GdTaO}_4$  laser crystal. *J. Lumin.* **2017**, 192, 555-61.