

A latest fluoride with excellent structural stiffness for ultra-efficient photoluminescence and specific four-peak emission temperature sensing

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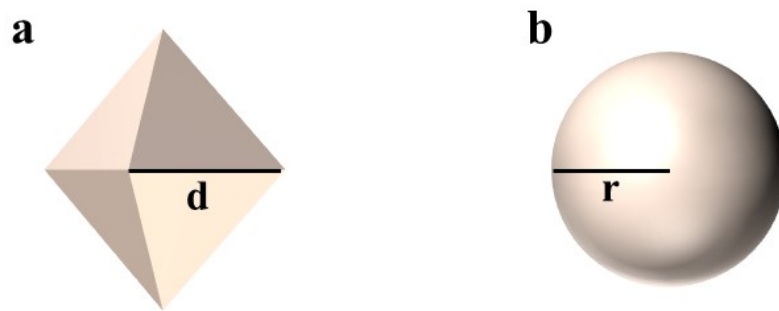


Figure S1 (a) the octahedral cones with edge length d . (b) traditional sphere with radius r .

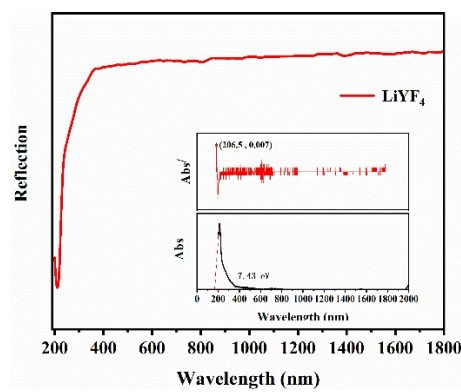


Figure S2 Diffuse reflectance spectrum and band gap calculation.

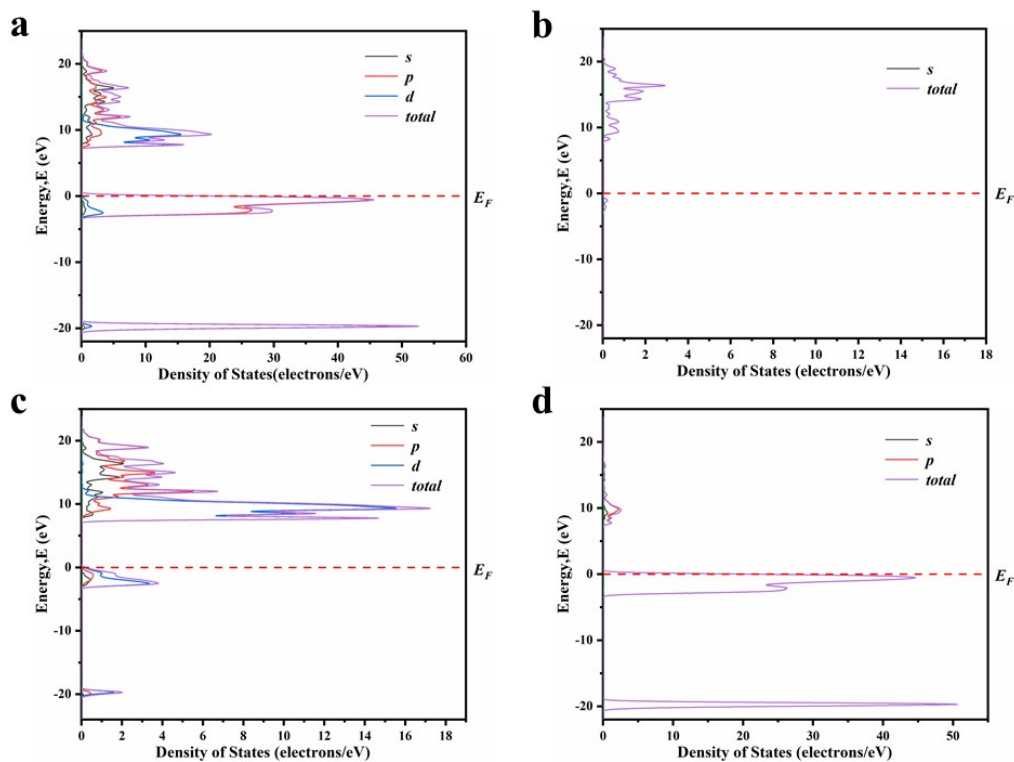


Figure S3 Calculated total DOS and atom-resolved PDOS of LiYF_4 : (a) total; (b) Li; (c) Y; (d) F.

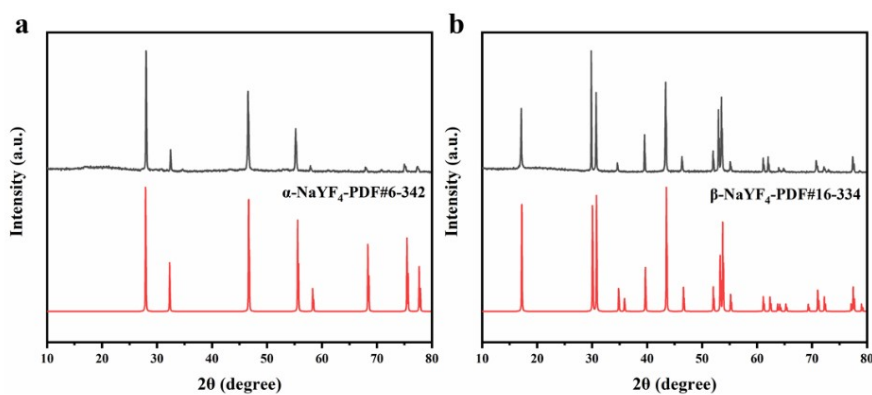


Figure S4 The XRD patterns of $\alpha\text{-NaYF}_4$ (a) and $\beta\text{-NaYF}_4$ (b).

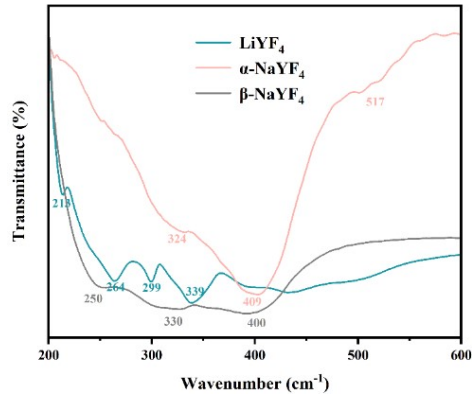


Figure S5 FTIR spectra of LiYF_4 , $\alpha\text{-NaYF}_4$ and $\beta\text{-NaYF}_4$.

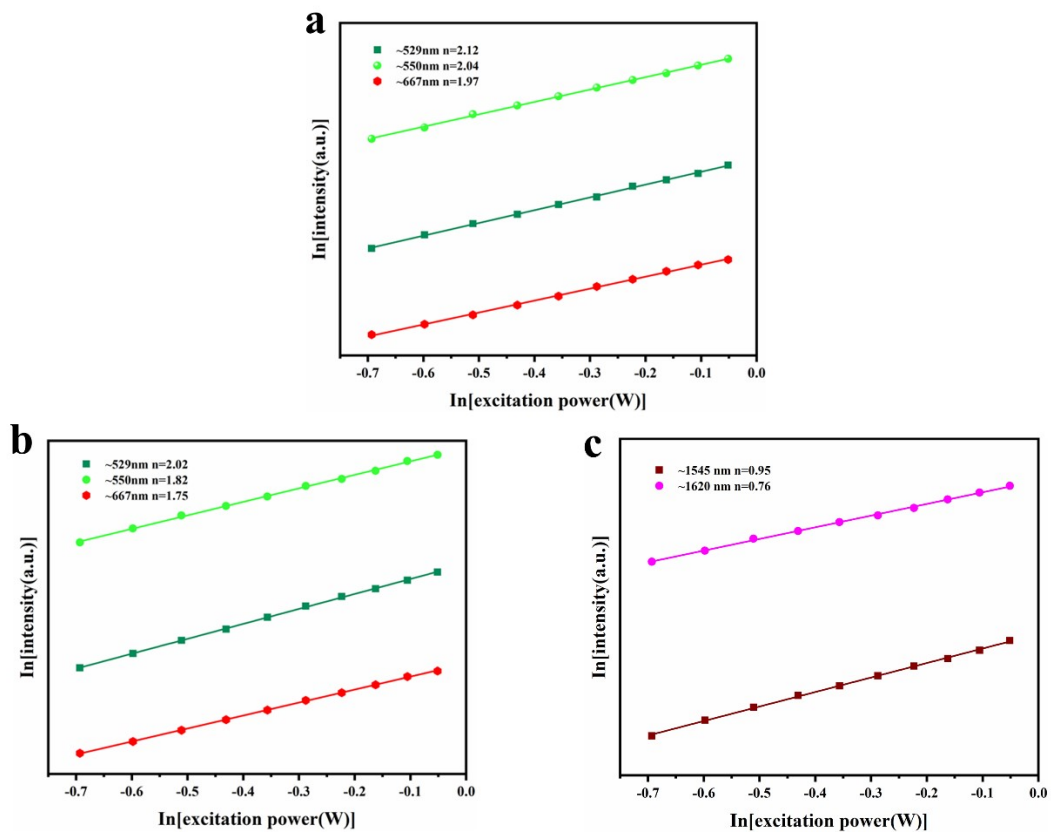


Figure S6 The relationship between $\ln(I)$ and $\ln(P)$ for $\text{LiYF}_4:1\%\text{Er}^{3+}$ under 980 nm (a) and 808 nm (b) excitation in the visible region and near infrared regions (c).

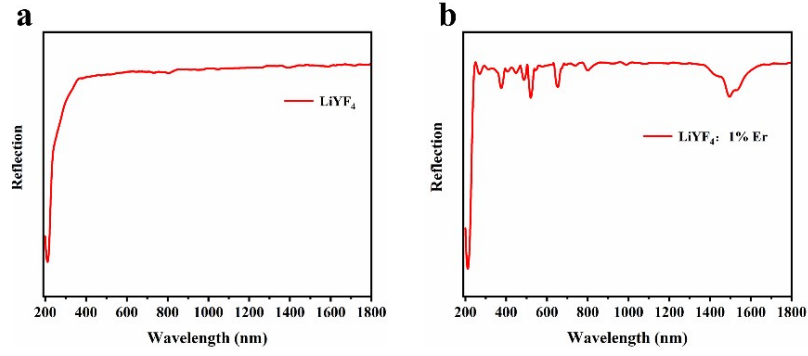


Figure S7 Diffuse reflectance spectrum of LiYF_4 host (a) and $\text{LiYF}_4:1\%\text{Er}$ (b).

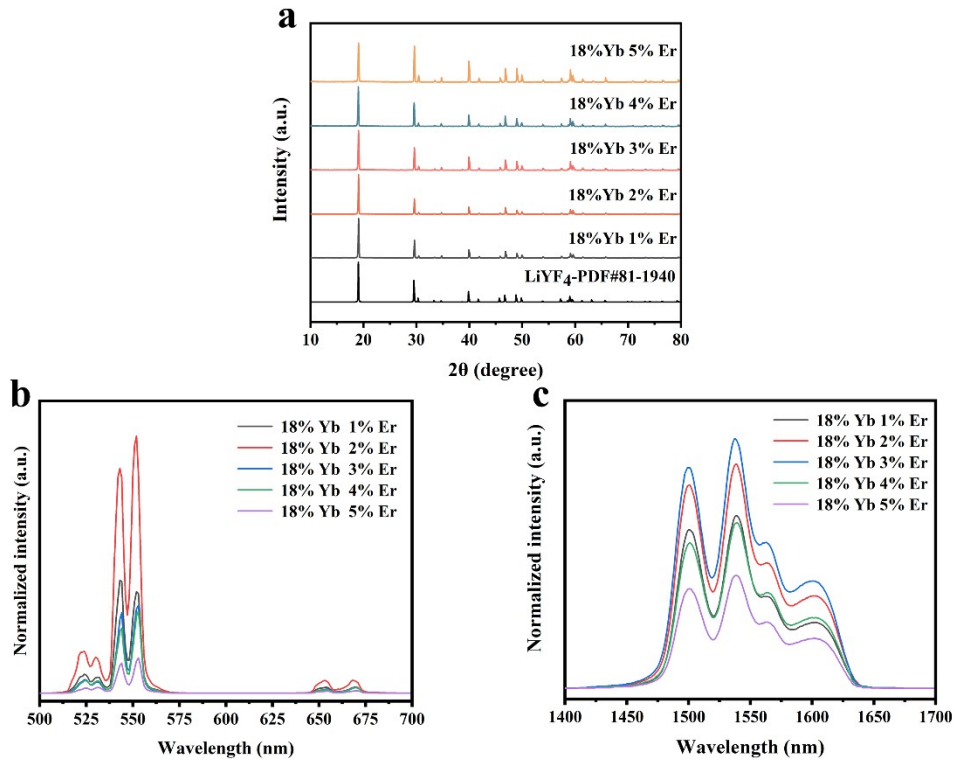


Figure S8 (a) The XRD patterns of $\text{LiYF}_4:18\%\text{Yb}^{3+}, x\%\text{Er}^{3+}$ ($x=1, 2, 3, 4, 5$) with the standard XRD data of LiYF_4 (DPF 81–1940). (b) Visible PL spectra and (c) NIR PL spectra of the $\text{LiYF}_4:18\%\text{Yb}^{3+}, x\%\text{Er}^{3+}$ ($x=1, 2, 3, 4, 5$) under 980 nm excitation.

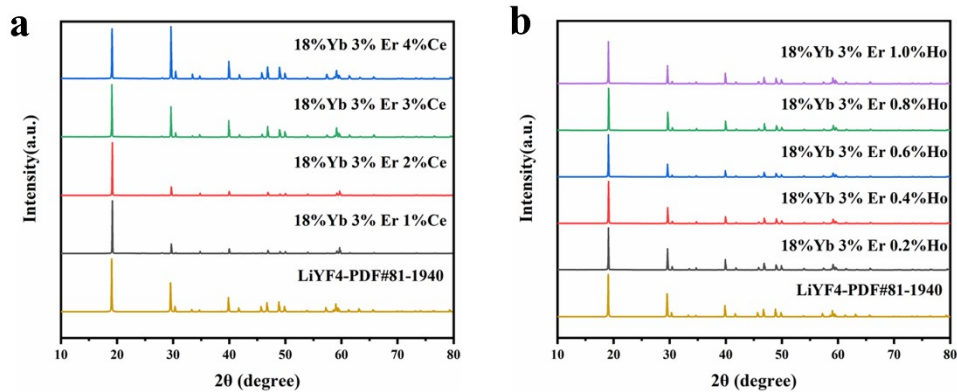


Figure S9 (a) The XRD patterns of LiYF_4 : 18% Yb^{3+} , 3% Er^{3+} , $x\%\text{Ce}^{3+}$ ($x=1, 2, 3, 4$) with the standard XRD data of tetragonal phase LiYF_4 (DPF 81–1940). (b) The XRD patterns of LiYF_4 : 18% Yb^{3+} , 3% Er^{3+} , $x\%\text{Ho}^{3+}$ ($x=0.2, 0.4, 0.6, 0.8, 1.0$) with the standard XRD data of tetragonal phase LiYF_4 (DPF 81–1940).

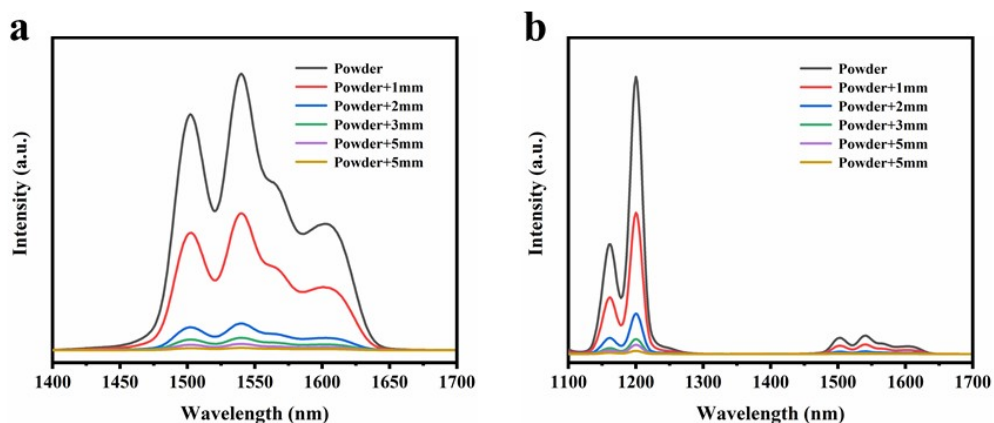


Figure S10 The PL spectra for the LiYF_4 : 18% Yb^{3+} , 3% Er^{3+} , 2% Ce^{3+} (a) and LiYF_4 : 18% Yb^{3+} , 3% Er^{3+} , 1% Ho^{3+} (b) with different depths of chicken breast.

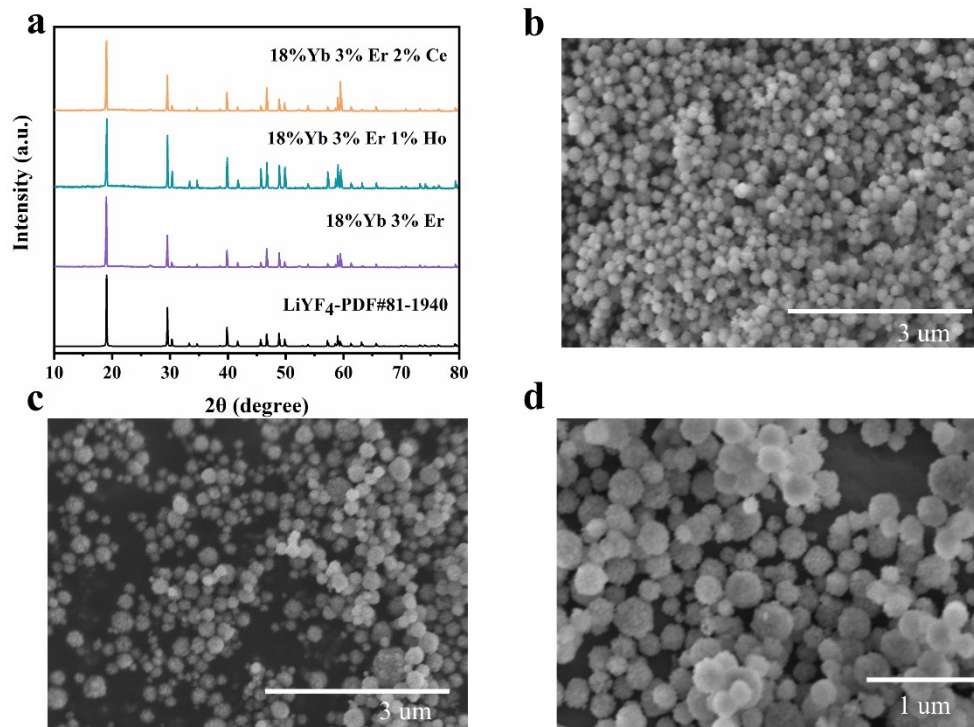


Figure S11 (a) The XRD patterns of LiYF₄:18%Yb³⁺, 3%Er³⁺, LiYF₄:18%Yb³⁺, 3%Er³⁺, 1%Ho³⁺ and LiYF₄:18%Yb³⁺, 3%Er³⁺, 2%Ce³⁺ with the standard XRD data of tetragonal phase LiYF₄(DPF 81–1940). SEM image of LiYF₄:18%Yb³⁺, 3%Er³⁺(b), LiYF₄:18%Yb³⁺, 3%Er³⁺, 1%Ho³⁺ (c) and LiYF₄:18%Yb³⁺, 3%Er³⁺, 2%Ce³⁺ (d).

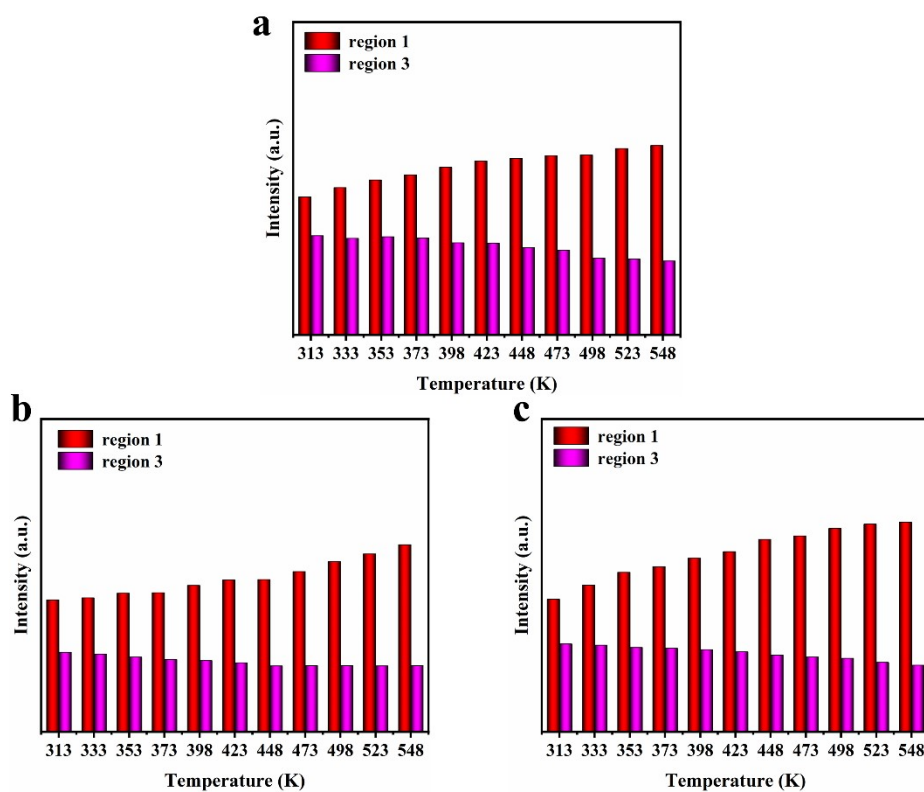


Figure S12 The integrated intensity summarizing of NIR-IIb (region 1.2.3) emission in LiYF₄:18%Yb³⁺, 3%Er³⁺ (a), LiYF₄:18%Yb³⁺, 3%Er³⁺, 0.2%Ho³⁺ (b) and LiYF₄:18%Yb³⁺, 3%Er³⁺, 2%Ce³⁺ (c) at different temperature;

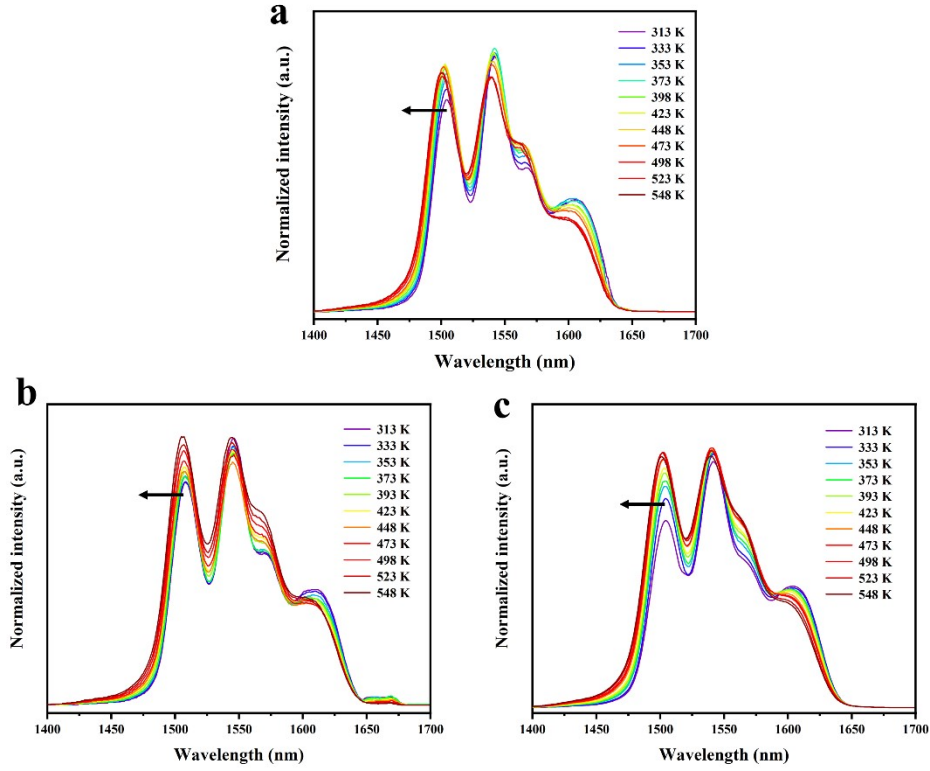


Figure S13 Temperature-dependent NIR-IIb emission spectra of LiYF₄:18% Yb³⁺, 3%Er³⁺ (a), LiYF₄:18%Yb³⁺, 3%Er³⁺, 0.2%Ho³⁺ (b) and LiYF₄:18%Yb³⁺, 3%Er³⁺, 2%Ce³⁺ (c)

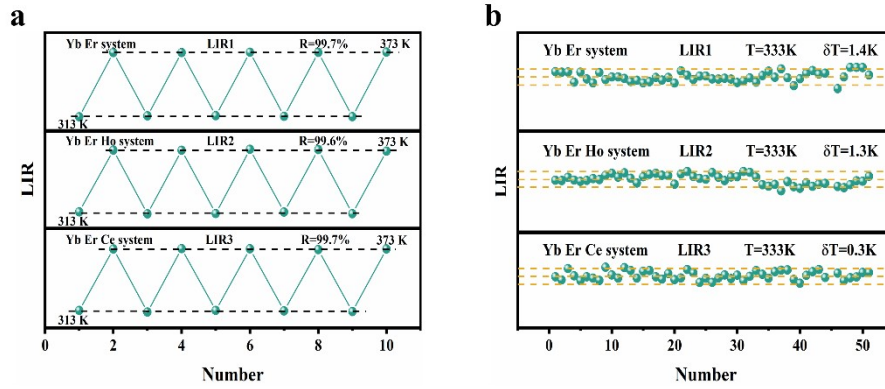


Figure S14 (a) LIR repeatability in 5 heating-cooling cycles. (b) LIR values were measured 50 times continuously at 333 K.

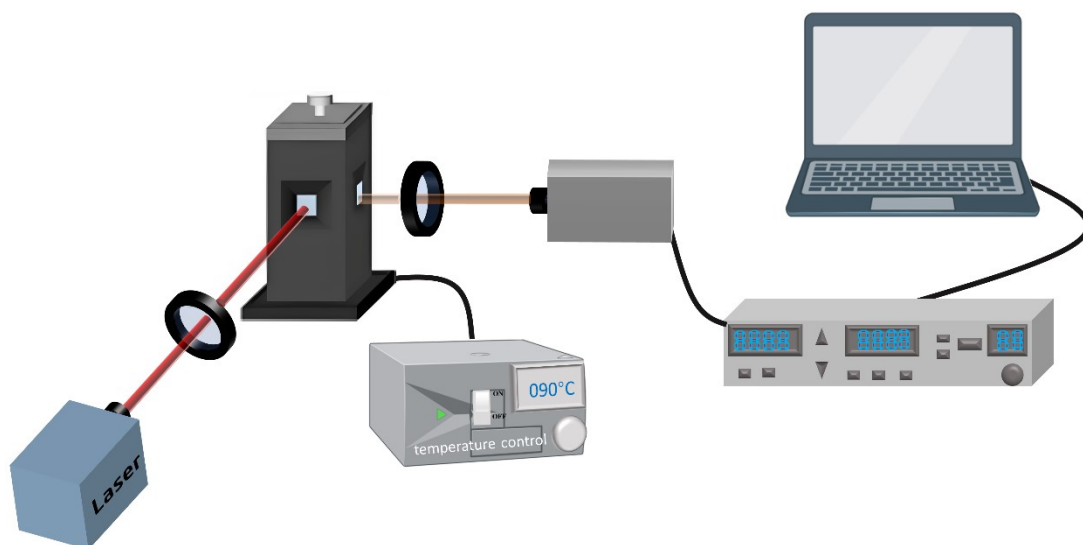


Figure S15 Schematic diagram of the experimental equipment for temperature sensing measurements.

Table S1:

The decomposition of each J in the C_4 point group ($\Gamma_j^\pm$ is the irreducible representation of $D_{j^\pm}$, $(\overline{\Gamma_i + \Gamma_j})$ represents two one-dimensional irreducible representations):

$D_0^\pm$	Γ_1
$D_1^\pm$	$\Gamma_1 + (\overline{\Gamma_3 + \Gamma_4})$
$D_2^\pm$	$\Gamma_1 + 2\Gamma_2 + (\overline{\Gamma_3 + \Gamma_4})$
$D_3^\pm$	$\Gamma_1 + 2\Gamma_2 + 2(\overline{\Gamma_3 + \Gamma_4})$
$D_4^\pm$	$3\Gamma_1 + 2\Gamma_2 + 2(\overline{\Gamma_3 + \Gamma_4})$
$D_5^\pm$	$3\Gamma_1 + 2\Gamma_2 + 3(\overline{\Gamma_3 + \Gamma_4})$
$D_6^\pm$	$3\Gamma_1 + 4\Gamma_2 + 3(\overline{\Gamma_3 + \Gamma_4})$
$D_7^\pm$	$3\Gamma_1 + 4\Gamma_2 + 4(\overline{\Gamma_3 + \Gamma_4})$
$D_8^\pm$	$5\Gamma_1 + 4\Gamma_2 + 4(\overline{\Gamma_3 + \Gamma_4})$
$D_{1/2}^\pm$	$(\overline{\Gamma_5 + \Gamma_6})$

Compatibility relationship between group C_{4h} and group C_4 :

Number of energy level splits of J energy levels in the point group:

J	0	1	2	3	4	5	6	7	8	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2	17/2
C ₄	1	2	4	5	7	8	10	11	13	1	2	3	4	5	6	7	8	9
C _{4h}																		