Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Design of Anti-thermal Quenching Pr^{3+}-doped Niobate Phosphor Based on Charge Transfer and Intervalence Charge Transfer Band Excitation-driven Strategy

Chunwei Yang,[a] Ning Guo,[a,*] Song Qu,[a] Qinchan Ma,[a] Jianxia Liu,[a] Shunyi Chen,[a] and Ruizhuo Ouyang[a],

[a] Department of Chemistry, University of Shanghai for Science and Technology, Shanghai 200093, P. R. China.

*Corresponding author: E-mail: guoning@usst.edu.cn

Contents

Part 1. Supporting Figures

Figure S1

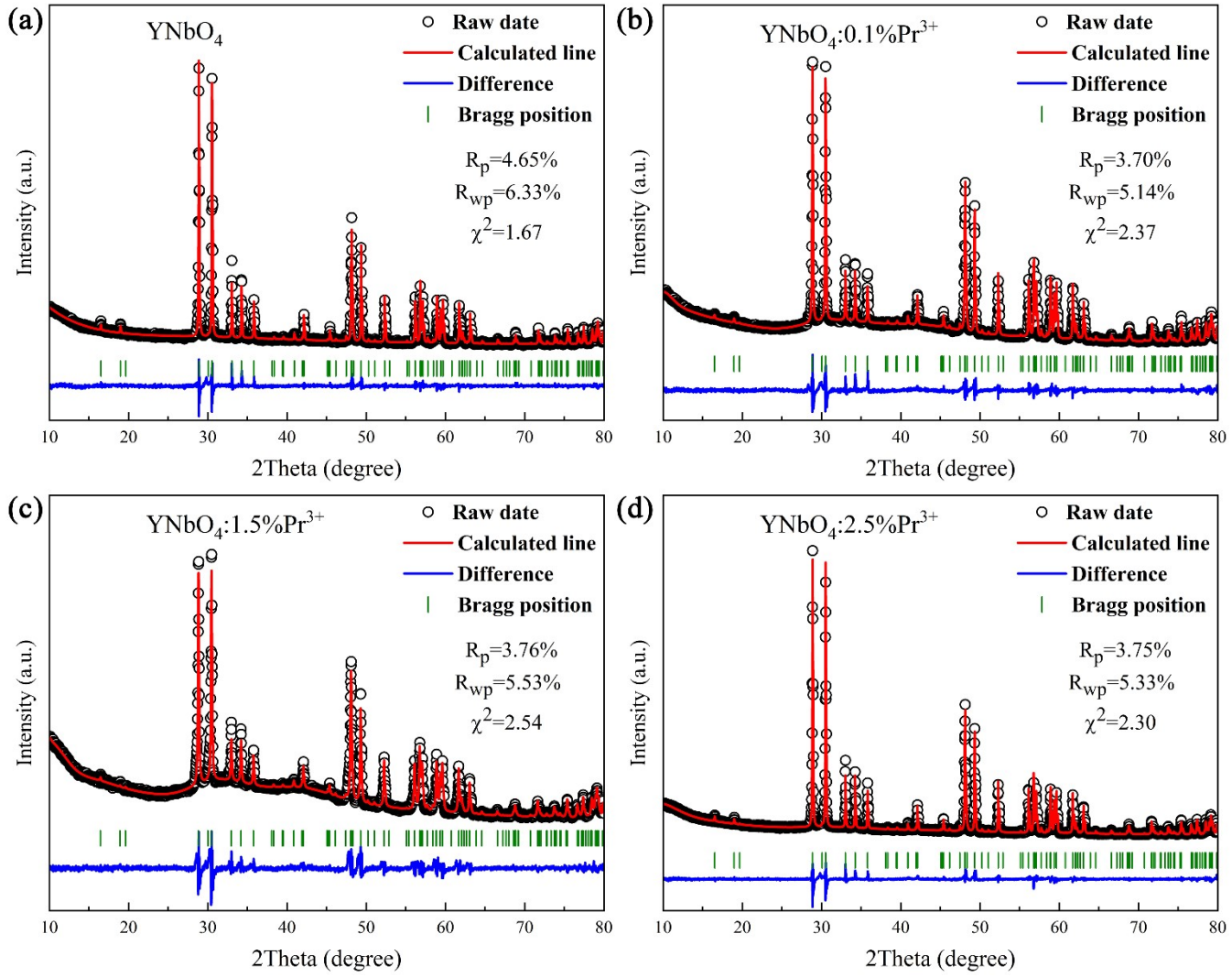

Figure S1. The Rietveld refinement plot of the X-ray diffraction pattern of $YNbO_4$:x%Pr^{3+} (x = 0, 0.1, 1.5, 2.5).

Figure S2

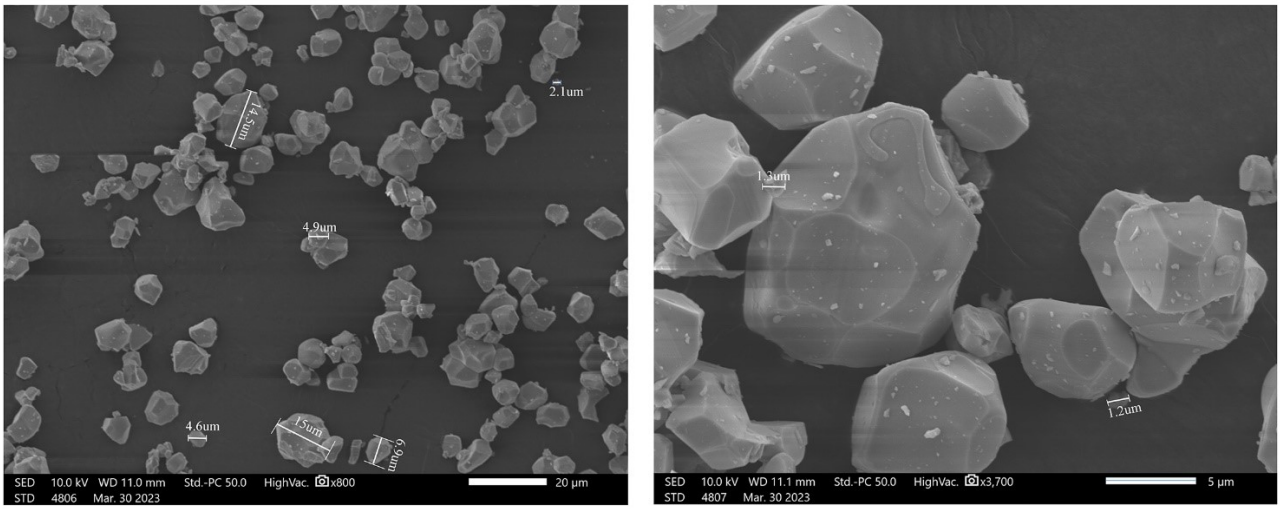

Figure S2. The SEM image of $YNbO_4$:0.5%Pr^{3+}.

Figure S3

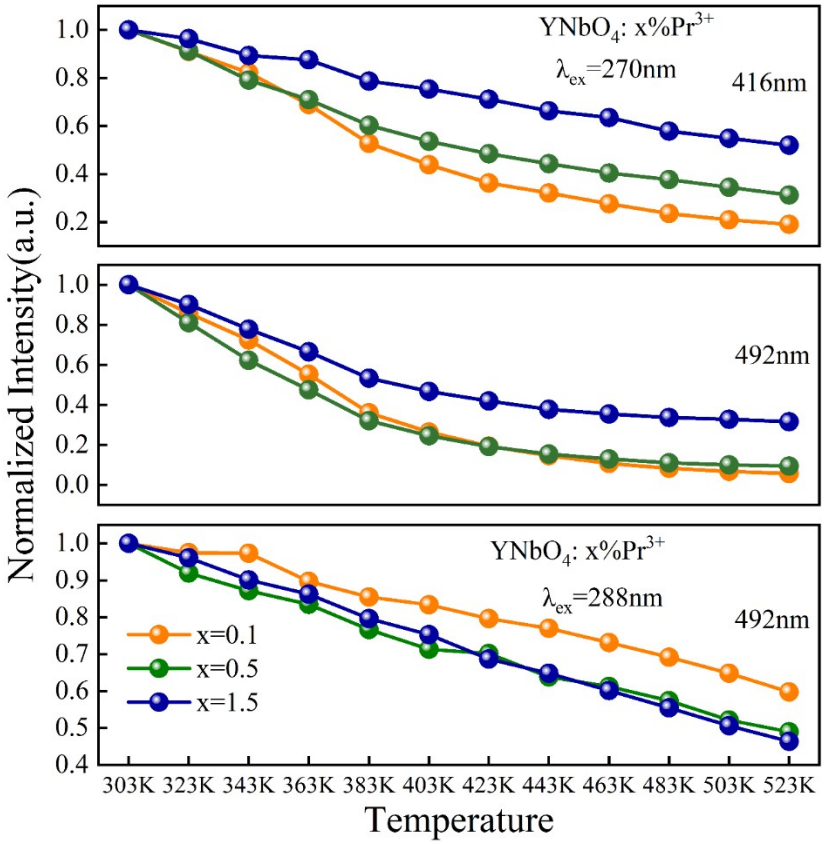

Figure S3. Temperature behavior of integrated intensity of matrix emission and $^3P_0$ emission of $YNbO_4$:x%Pr^{3+} (x = 0.1, 0.5, 1.5) under excitation of 270 nm and 288 nm.

Figure S4

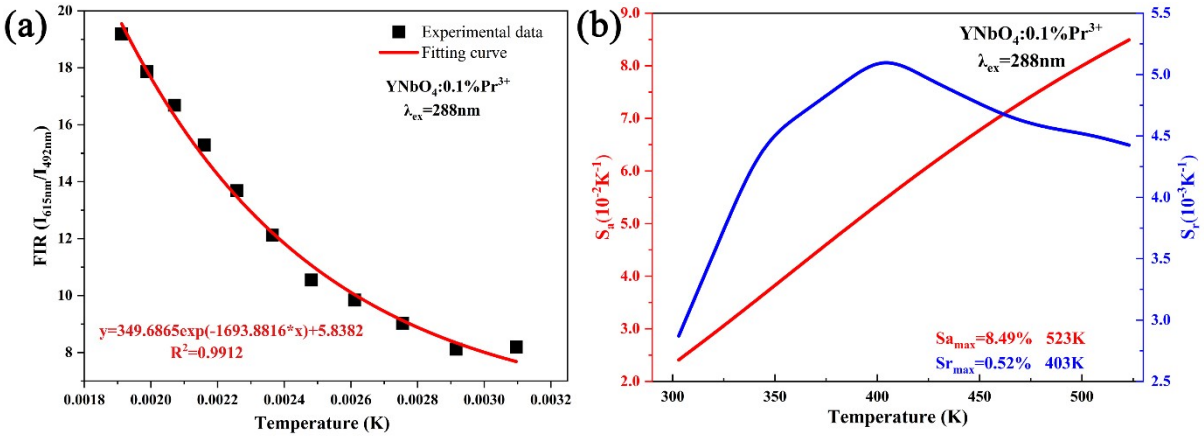

Figure S4. (a) Experimental data and fitted plots of FIR (I_{615} nm/I_{492} nm) versus temperature in the range of 303–523 K for $YNbO_4$:0.1%Pr^{3+}. (b) Plot of absolute sensitivity S_a and relative sensitivity S_r vs. temperature (303–523 K) for $YNbO_4$:0.1%Pr^{3+} under excitation at 288 nm.

Figure S5

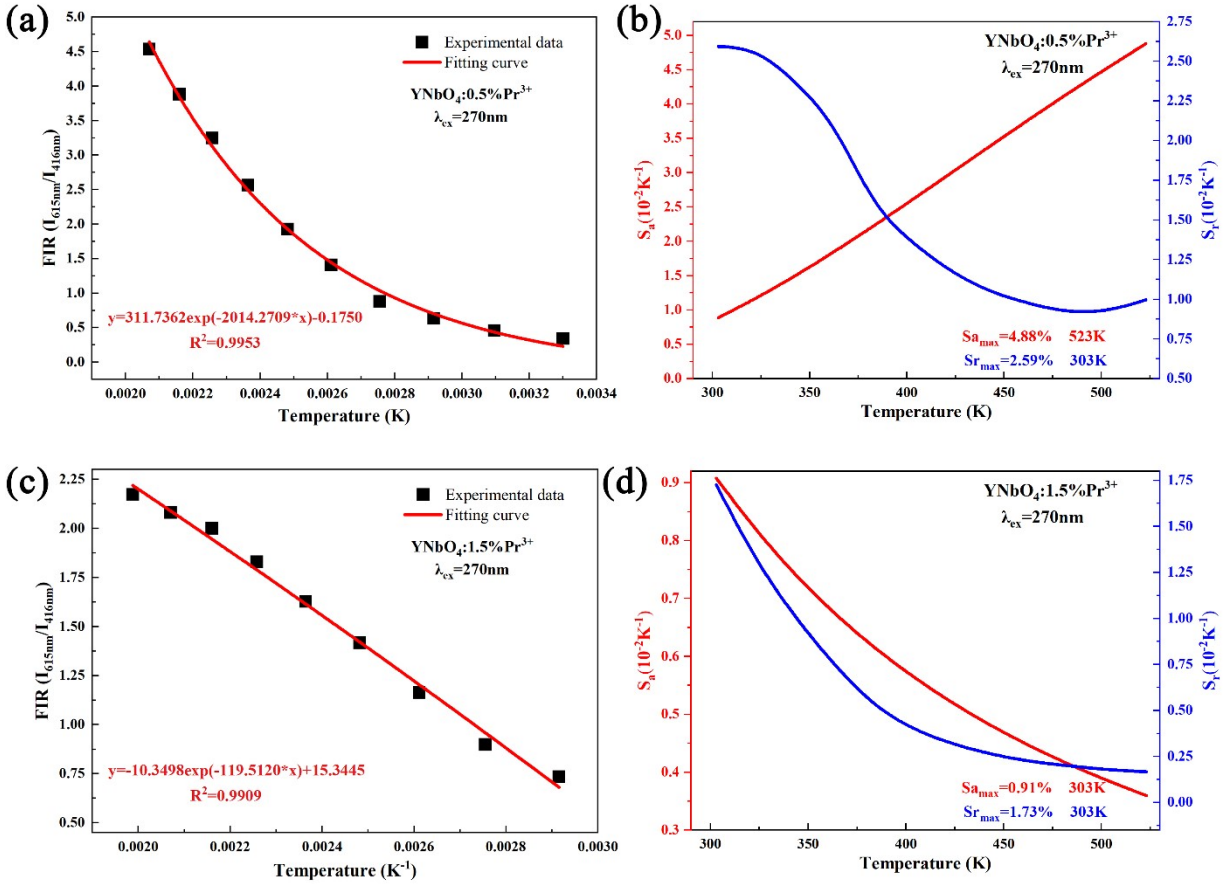

Figure S5. (a) and (c) Experimental data and fitted curves of FIR (I_{615} nm/I_{416} nm) vs. temperature for $YNbO_4$:x%Pr^{3+} (x = 0.5, 1.5) in the range of 303–523 K. (b)and (d) Plot of absolute sensitivity S_a and relative sensitivity S_r vs. temperature (303–523 K) for $YNbO_4$:x%Pr^{3+} (x = 0.5, 1.5) under excitation at 270 nm.

Figure S6

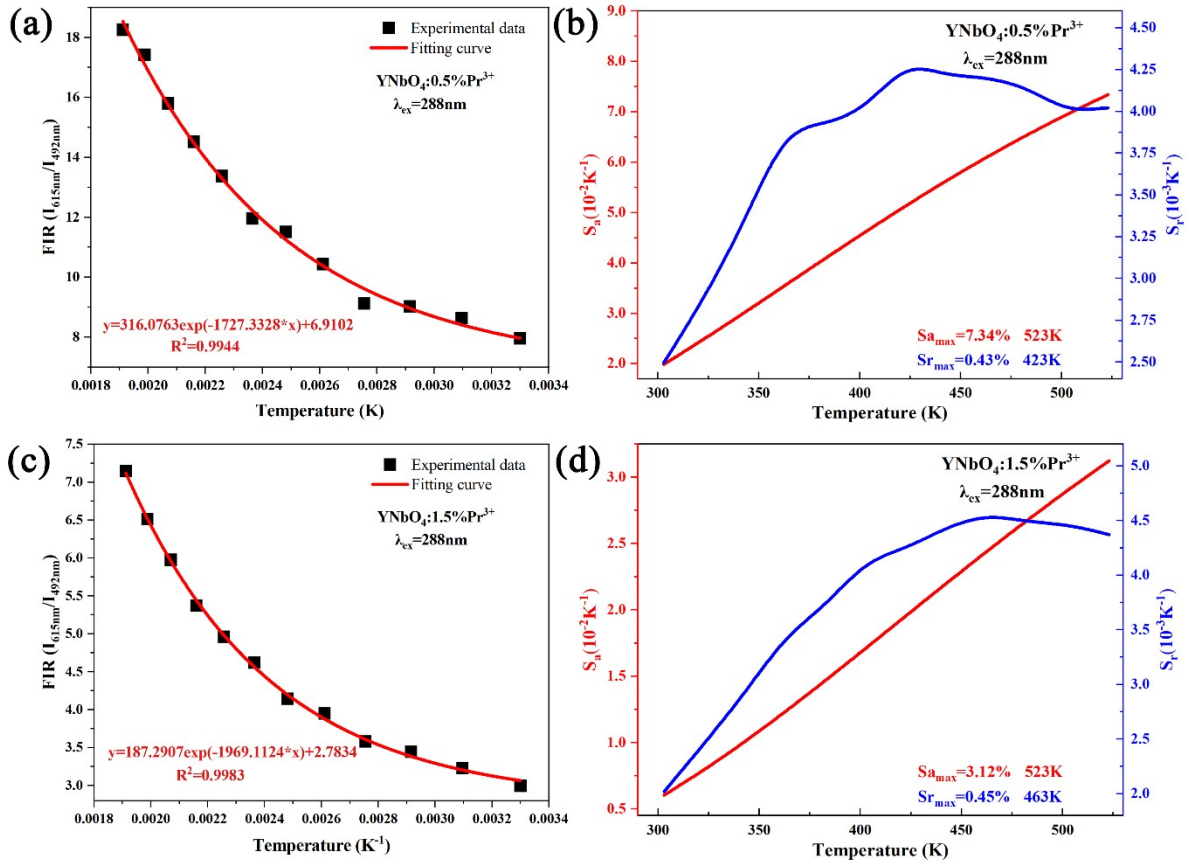

Figure S6. (a) and (c) Experimental data and fitted curves of FIR (I_{615} nm/I_{492} nm) vs. temperature for $YNbO_4$:x%Pr^{3+} (x = 0.5, 1.5) in the range of 303–523 K. (b) and (d) Plot of absolute sensitivity S_a and relative sensitivity S_r vs. temperature (303–523 K) for $YNbO_4$:x%Pr^{3+}(x = 0.5, 1.5) under excitation at 288 nm.

Figure S7

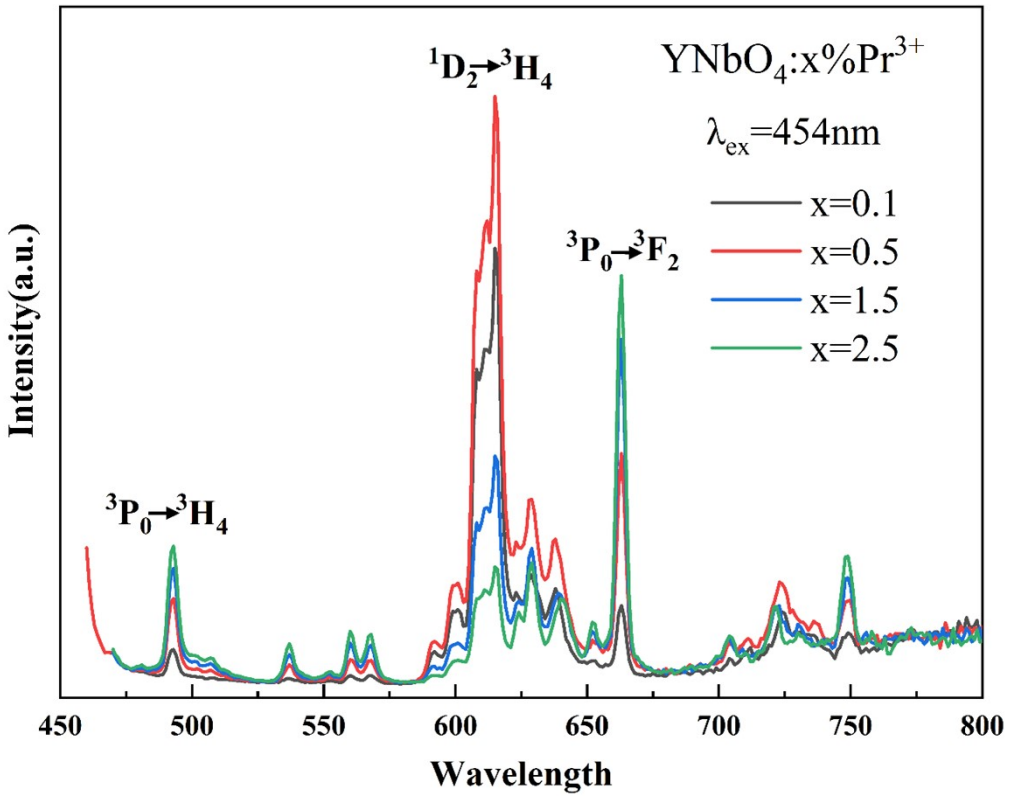

Figure S7. PL spectrum of $YNbO_4:x\%Pr^{3+}$ (x = 0, 0.1, 0.5, 1.5, 2.5) phosphors excited at 454 nm.

Figure S8

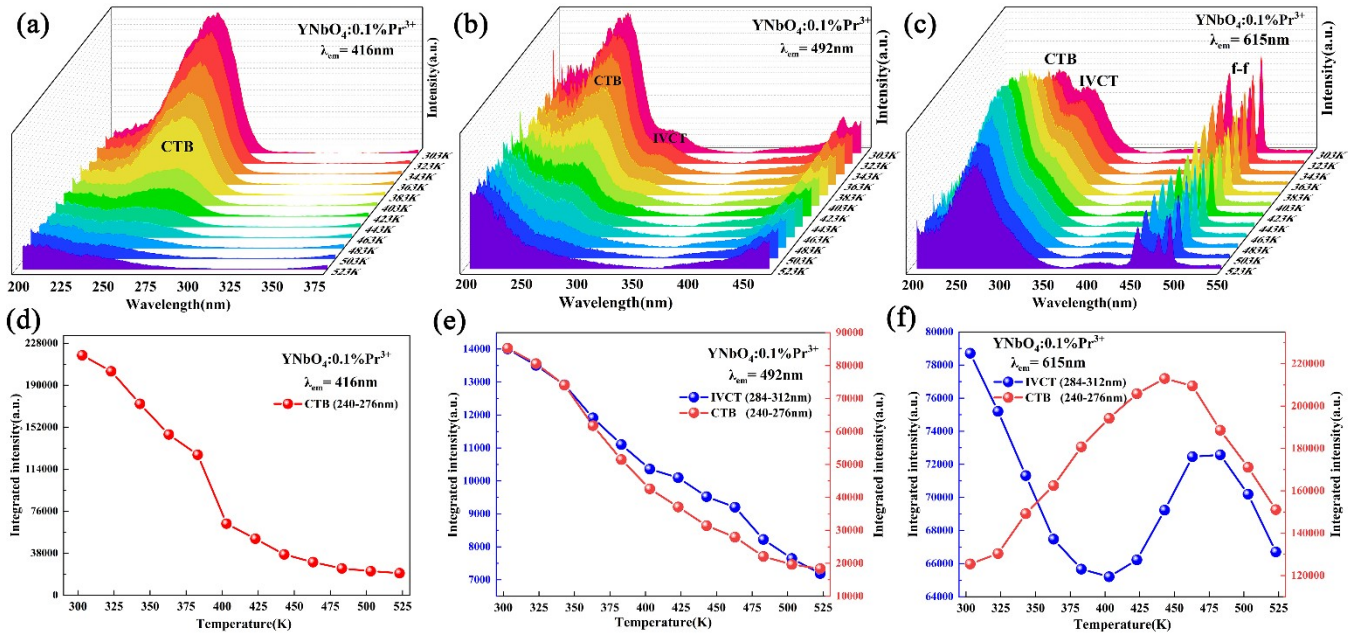

Figure S8. (a) Temperature-dependent PLE spectra of $YNbO_4$:0.1%Pr^{3+} phosphor under the monitoring of 416 nm, (b) 492 nm and (c) 615 nm. (d-f) Temperature-dependent curve of luminescence integrated intensity in the PLE spectrum of $YNbO_4$:0.1%Pr^{3+} phosphor.

Figure S9

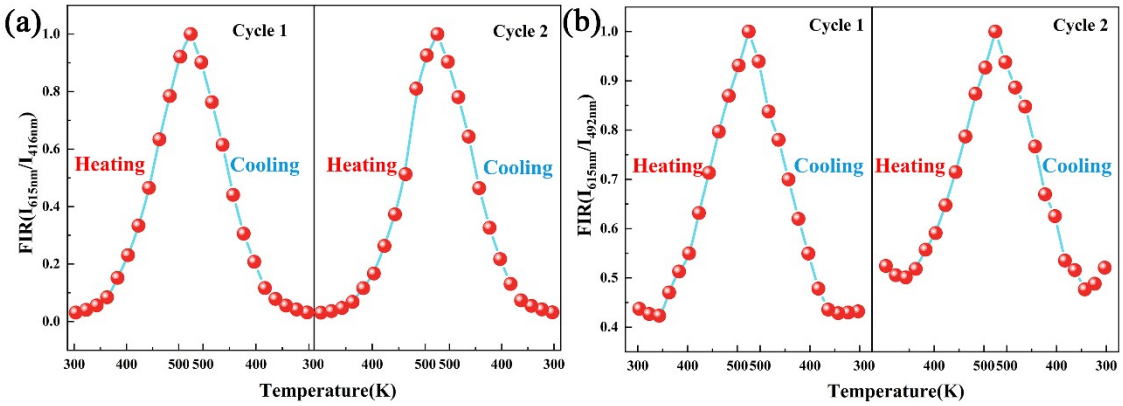

Figure S9. (a) FIR value of $YNbO_4$:0.1%Pr^{3+} phosphor in temperature-cycle test under excitation of 270 nm and (b) 288 nm.

Figure S10

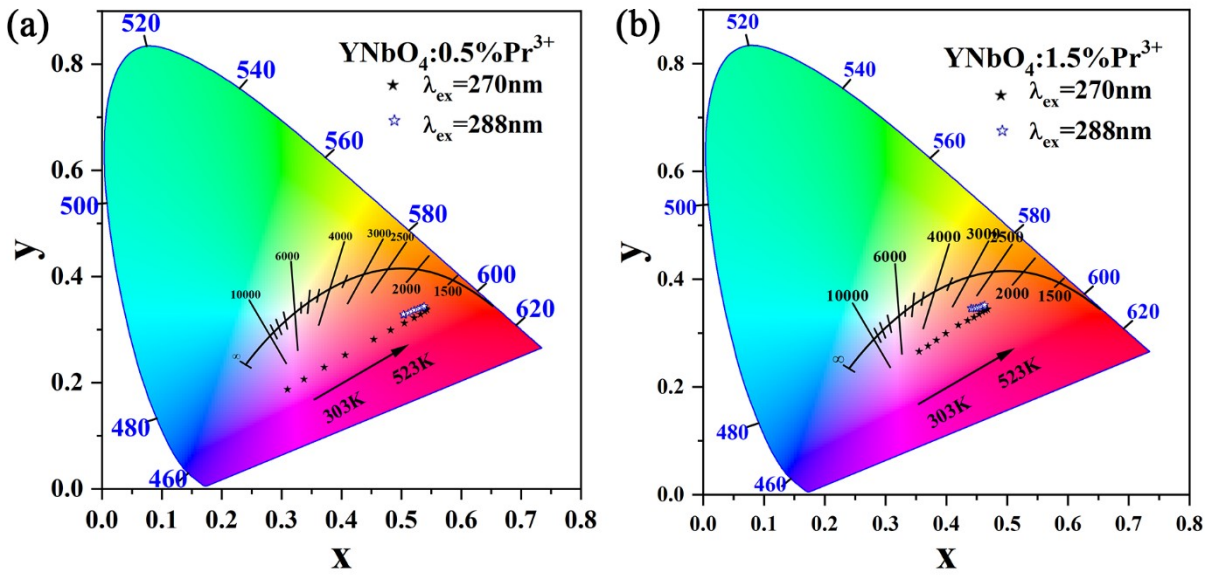

Figure S10. (a) and (b) CIE chromaticity diagram and photograph of $YNbO_4$:x%Pr^{3+} (x = 0.5, 1.5) at different temperatures under 270 nm and 288 nm excitation.

Part 2. Supporting Tables

Table S1

Table S1. Refinement results of the atomic coordinates of $YNbO_4$:x%Pr^{3+} (x = 0, 0.1, 0.5, 1.5, 2.5).

Formula	Atom	x	y	z	Occ.	Mult
$YNbO_4$	Y1	0.0000	0.6219(3)	0.25000	1.0000	4
	Nb1	0.0000	0.1437(23)	0.25000	1.0000	4
	O1	0.2512(25)	0.9409(8)	0.3451(29)	1.0000	8
	O2	0.3451(29)	0.2872(7)	0.2970(3)	1.0000	8
$YNbO_4$:0.1%Pr^{3+}	Y1	0.00000	0.6213(4)	0.25000	0.9990	4
	Pr1	0.00000	0.6213(4)	0.25000	0.0010	4
	Nb1	0.00000	0.1432(24)	0.25000	1.0000	4
	O1	0.2661(27)	0.0372(8)	0.3555(30)	1.0000	8
	O2	0.2956(28)	0.2875(8)	0.282(4)	1.0000	8
$YNbO_4$:0.5%Pr^{3+}	Y1	0.00000	0.6222(4)	0.25000	0.9950	4
	Pr1	0.00000	0.6000(5)	0.25000	0.0050	4
	Nb1	0.00000	0.1442(20)	0.25000	0.9702	4
	O1	0.2692(18)	0.0344(6)	0.3642(21)	1.017(15)	8
	O2	0.3081(17)	0.2865(6)	0.2772(28)	1.056(13)	8
$YNbO_4$:1.5%Pr^{3+}	Y1	0.00000	0.6224(7)	0.25000	0.9850	4
	Pr1	0.00000	0.625(25)	0.25000	0.0150	4
	Nb1	0.00000	0.1440(4)	0.25000	1.0000	4
	O1	0.266(4)	0.0337(13)	0.3560(4)	1.0000	8
	O2	0.295(4)	0.2863(12)	0.271(7)	1.0000	8
$YNbO_4$:2.5%Pr^{3+}	Y1	0.00000	0.6210(7)	0.25000	0.9750	4
	Pr1	0.00000	0.6200(20)	0.25000	0.0250	4
	Nb1	0.00000	0.1436(18)	0.25000	1.0026	4
	O1	0.2525(23)	0.0373(7)	0.3377(26)	0.9224	8
	O2	0.2929(21)	0.2849(6)	0.2957(29)	0.9669	8

Table S2

Table S2. Refinement results of the atomic coordinates of $YNbO_4$:x%Pr^{3+} (x = 0, 0.1, 0.5, 1.5, 2.5).

parameter	space group	a(Å)	b(Å)	c(Å)	α = γ(°)	β(°)	V(Å^3)
$YNbO_4$	C12/c1(15)	7.0358	10.94628	5.2972	90	134.0726	293.1080
$YNbO_4$:0.1%Pr^{3+}	C12/c1(15)	7.0354	10.94520	5.2967	90	134.0753	293.1080
$YNbO_4$:0.5%Pr^{3+}	C12/c1(15)	7.0368	10.94805	5.2981	90	134.0765	293.2279
$YNbO_4$:1.5%Pr^{3+}	C12/c1(15)	7.038	10.95050	5.2992	90	134.0870	293.3720
$YNbO_4$:2.5%Pr^{3+}	C12/c1(15)	7.041	10.95654	5.3021	90	134.0909	293.8038

Table S3

Table S3. Temperature sensing performances of several typical temperature sensors.

Phosphors	λ_{ex}(nm)	Temperature range(K)	Mode	Max. $S_a(K^{-1})$	Max. $S_r(\%K^{-1})$	Ref.
$Gd_2ZnTiO_6:Pr^{3+}$	300	293-433	FIR	0.63	1.67	52
$Ba_{0.995}TiO_3:Pr^{3+}$	370	313-413	FIR	0.0575	2.77	53
$YNbO_4:Pr^{3+},Tb^{3+}$	295	298-538	FIR	0.0125	1.01	54
$CaMoO_4:Pr^{3+}$	279	303-573	FIR	0.01684	2.216	55
$CaWO_4:Pr^{3+}$	290/450	303-573	FIR	/	1.5	56
$YNbO_4:Pr^{3+}$	270	303-523	FIR	0.0426	3.74	This work
$YNbO_4:Pr^{3+}$	288	303-523	FIR	0.0849	0.52	This work