Supplementary Information

Enhancing upconversion luminescence via intermediate state in double perovskite phosphor: three-mode optical thermometry with python-assisted validation

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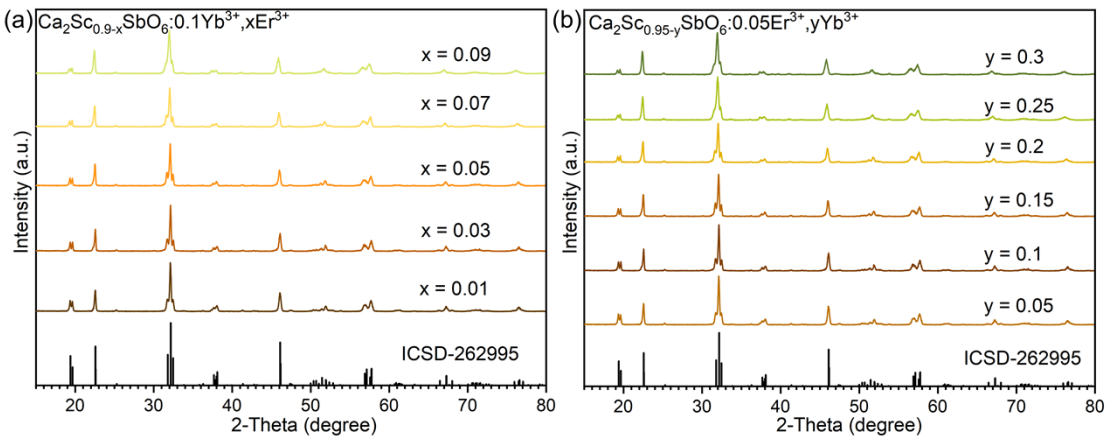

Fig. S1. XRD patterns of (a)$Ca_2Sc_{0.9-x}SbO_6$:$0.1Yb^{3+}$,xEr^{3+} (x = 0.01–0.09) and (b)$Ca_2Sc_{0.95-y}SbO_6$:$0.05Er^{3+}$,yYb^{3+} (y = 0.05–0.3).

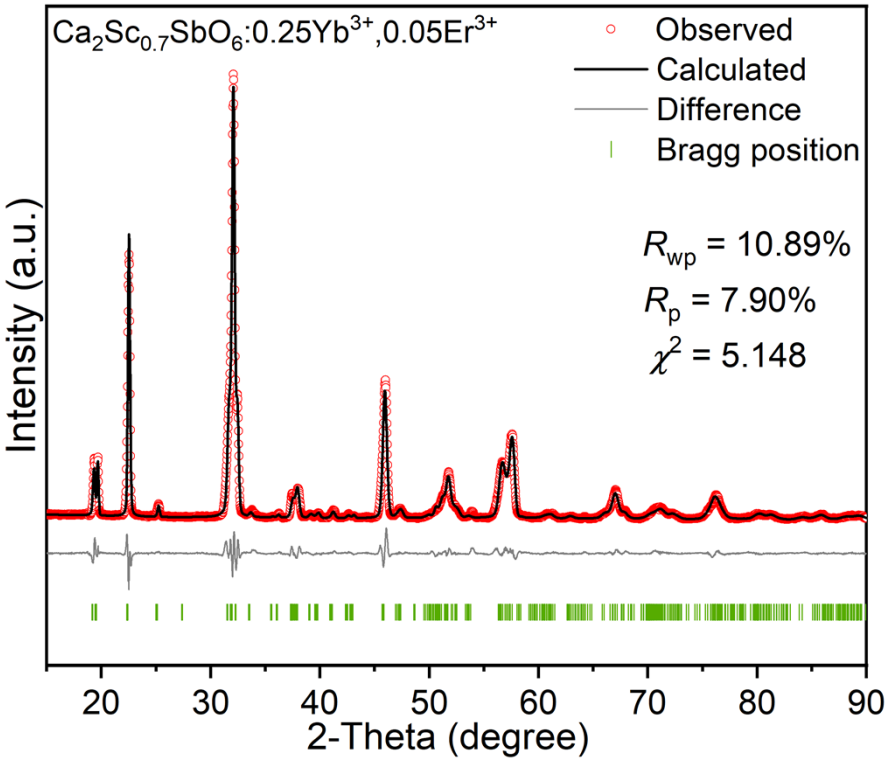

Fig. S2. Rietveld refinement of $Ca_2Sc_{0.7}SbO_6$:$0.25Yb^{3+}$,$0.05Er^{3+}$.

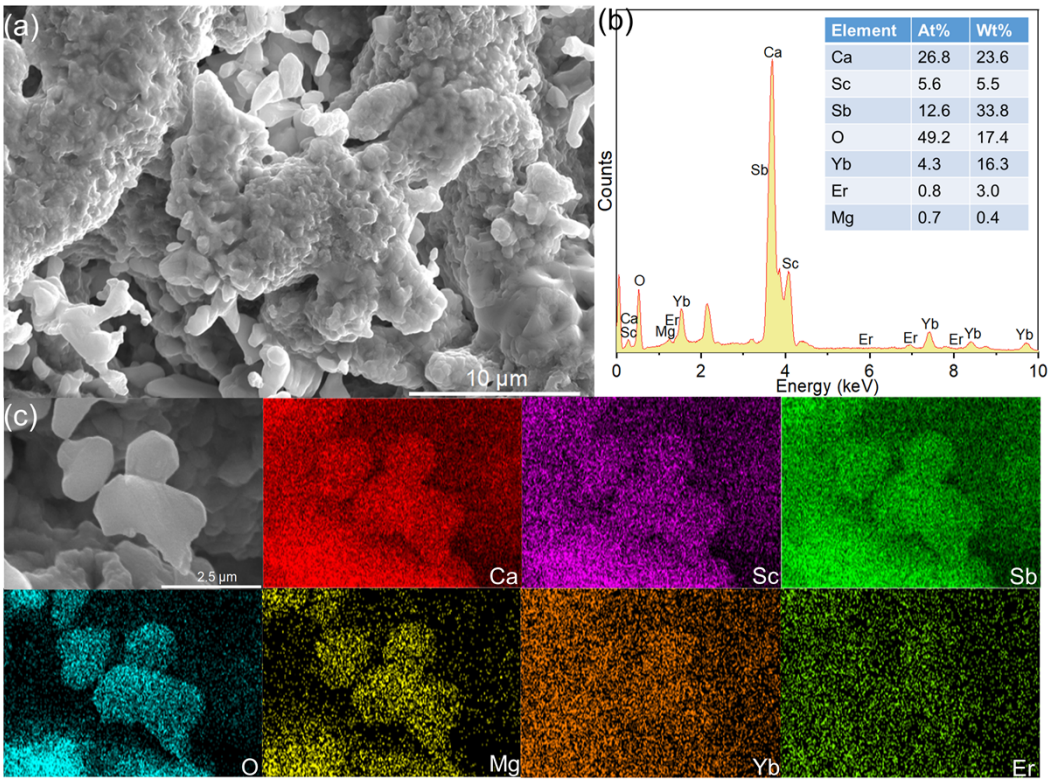

Fig. S3. (a) SEM image, (b) EDS and (c) the corresponding element mappings of the $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$.

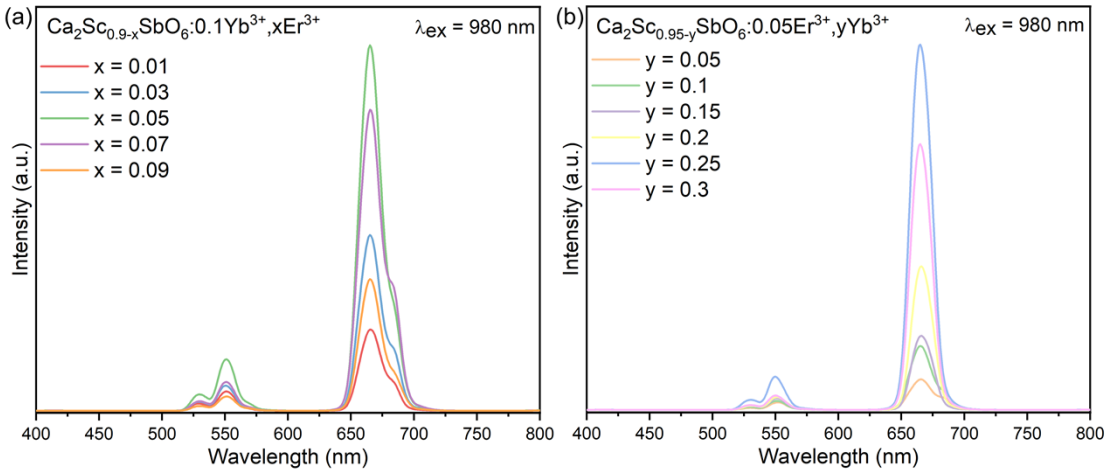

Fig. S4. UC spectra of (a) $Ca_2Sc_{0.9-x}SbO_6$:0.1Yb^{3+},xEr^{3+} (x = 0.01–0.09) and (b) $Ca_2Sc_{0.95-y}SbO_6$:0.05Er^{3+},yYb^{3+} (y = 0.05–0.3) under 980 nm laser excitation.

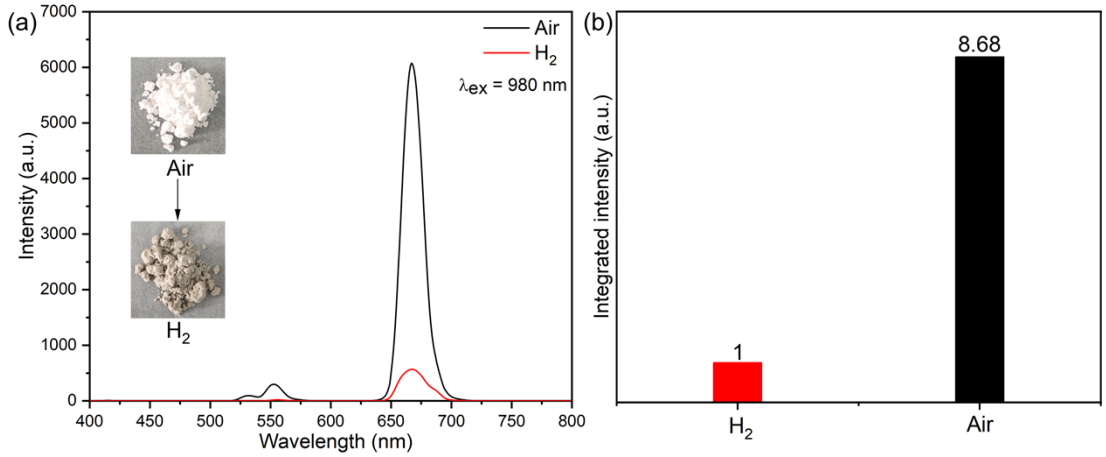

Fig. S5. (a) UC spectra in different atmospheres and (b) integrated intensity histogram of $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$.

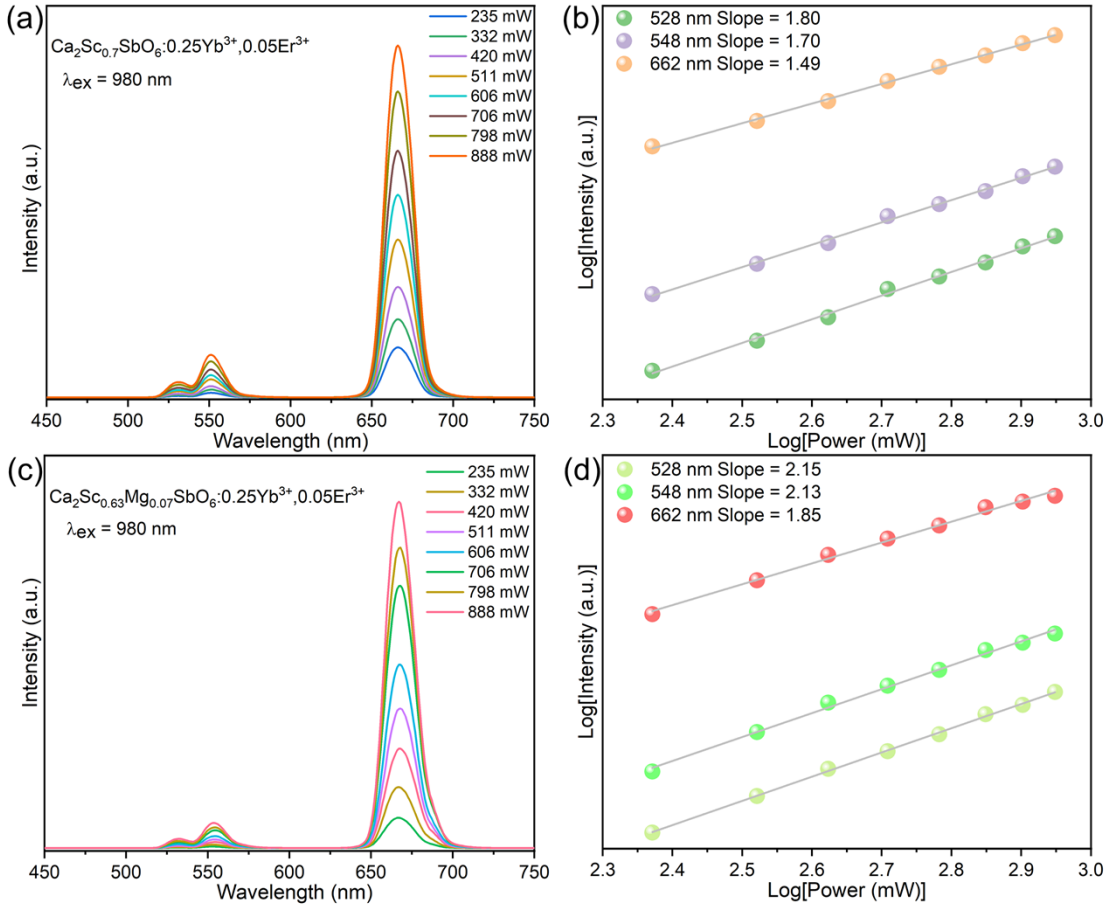

Fig. S6. Pump power-dependent UC spectra of (a) $Ca_2Sc_{0.7}SbO_6$:0.25Yb^{3+},0.05Er^{3+} and (c) $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$. Dependence of Log *I* on Log *P* for 528, 548, and 662 nm of (b) $Ca_2Sc_{0.7}SbO_6$:0.25Yb^{3+},0.05Er^{3+} and (d) $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$.

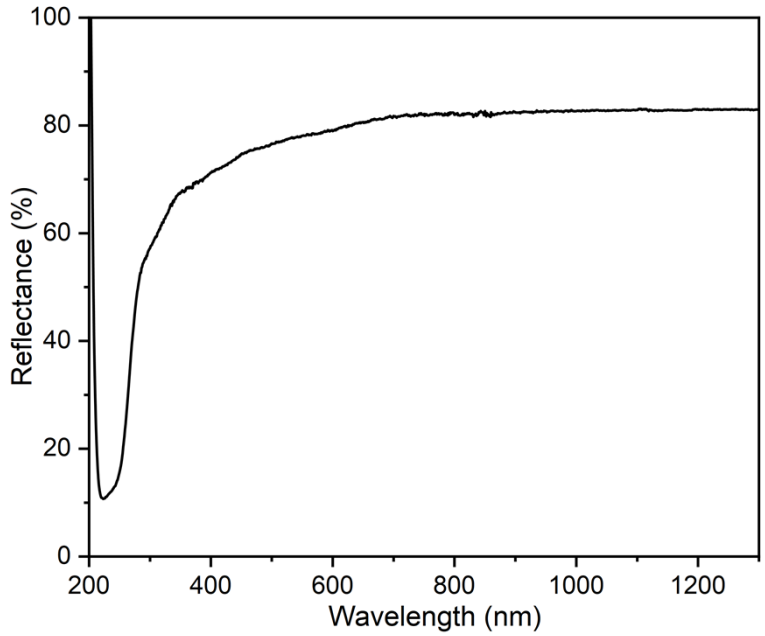

Fig. S7. Diffuse reflectance spectrum of Ca_2ScSbO_6.

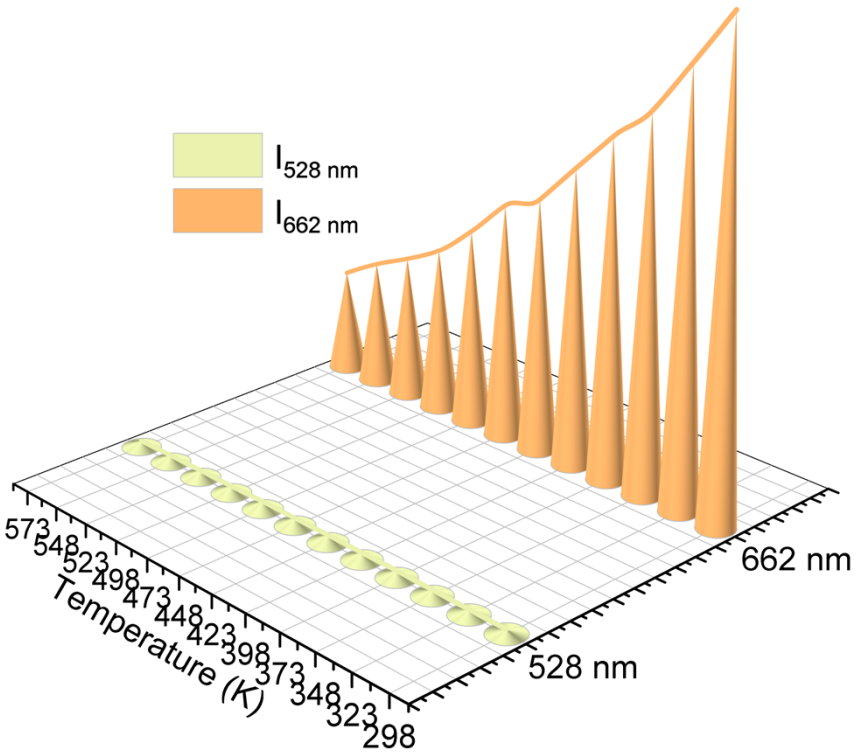

Fig. S8. Intensities of 528 nm and 662 nm versus temperature.

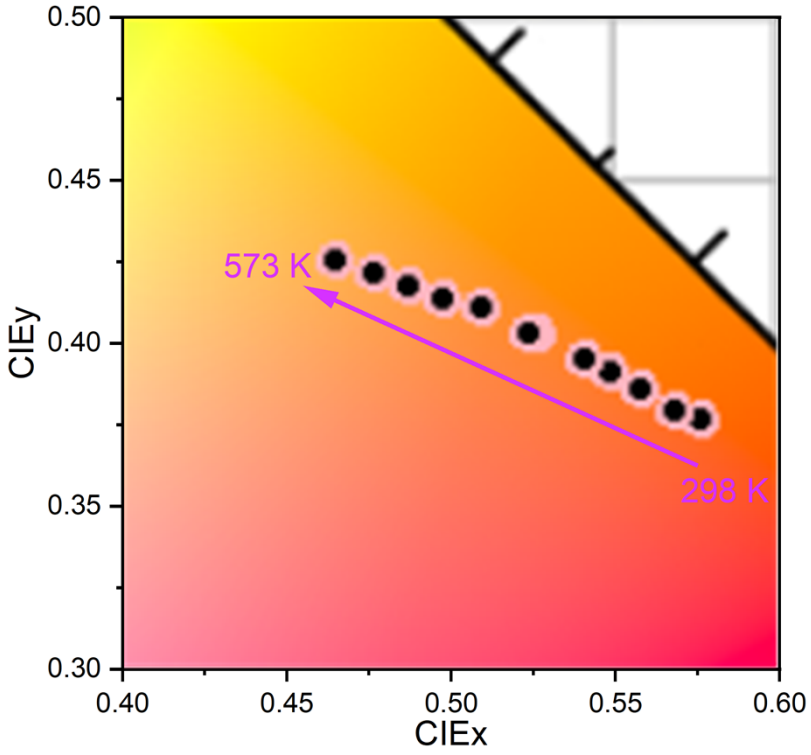

Fig. S9. CIE chromaticity coordinates for temperature range from 298 to 573K.

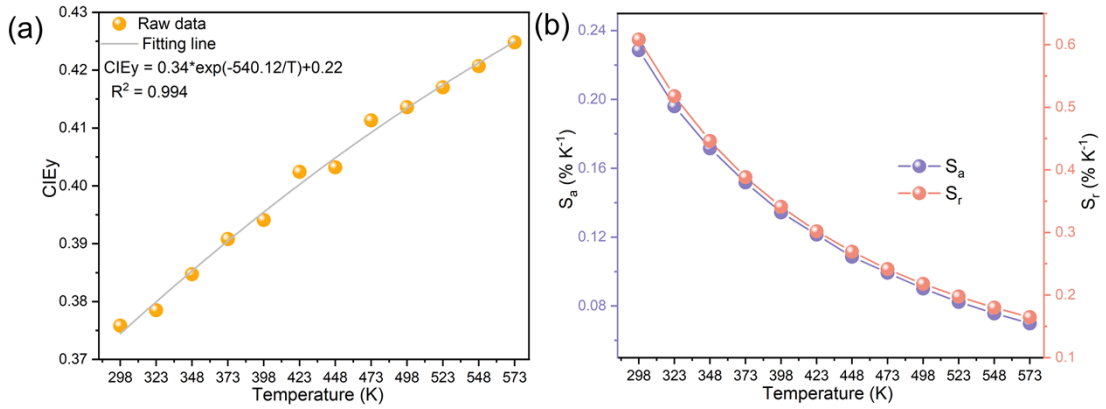

Fig. S10. (a) CIEy versus temperature. (b) S_a and S_r versus temperature.

Table S1

Lattice parameters and structural refinement of the $Ca_2Sc_{0.7}SbO_6$:0.25Yb^{3+},0.05Er^{3+} sample.

Phosphor	$Ca_2Sc_{0.7}SbO_6$:0.25Yb^{3+},0.05Er^{3+}				
Space group	*P*121/n1				
Cell parameters	*a* = 5.533489 Å, *b* = 5.663806 Å, *c* = 7.921733 Å, and *V* = 248.269 Å^3				
Atom	site	*x*	*y*	*z*	Occupancy
Ca	4e	0.021242	0.055381	0.244881	1
Sb	2c	0	0.5	0	1
Sc	2d	0.5	0	0	0.7757
Yb	2d	0.5	0	0	0.2243
O1	4e	0.314749	0.301903	0.057433	0.9978
O2	4e	0.285476	0.279853	0.439367	0.8846
O3	4e	0.900199	0.486997	0.234794	0.9701
Oxygen Vacancy	4.92%				

Note: Since the Er^{3+} concentration is very low (0.05 of the Sc^{3+} site), it is not included in the refinement.

Table S2

Lattice parameters and structural refinement of the $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$.

Phosphor	$Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$				
Space group	*P*121/n1				
Cell parameters	*a* = 5.525458 Å, *b* = 5.657392 Å, *c* = 7.898575 Å, and *V* = 246.906 Å^3				
Atom	site	*x*	*y*	*z*	Occupancy
Ca	4e	0.006579	0.051228	0.246184	1.0752
Mg	4e	0.006579	0.051228	0.246184	-0.0752
Sb	2c	0	0.5	0	1
Sc	2d	0.5	0	0	0.7273
Yb	2d	0.5	0	0	0.2119
Mg	2d	0.5	0	0	0.0608
O1	4e	0.306319	0.300459	0.040992	0.9210

O2	4e	0.288603	0.297456	0.424062	0.9184
O3	4e	0.903164	0.474923	0.229862	0.9293
Oxygen Vacancy			7.71%		

Table S3
Chromaticity shift (ΔE_s) of $Ca_2Sc_{0.63}Mg_{0.07}SbO_6$:0.25$Yb^{3+}$,0.05$Er^{3+}$ in response to temperature.

Temperature (K)	CIE (x, y)	ΔE_s
323	(0.5695, 0.3785)	0.011
348	(0.5589, 0.3847)	0.027
373	(0.5491, 0.3908)	0.042
398	(0.5410, 0.3941)	0.053
423	(0.5267, 0.4024)	0.073
448	(0.5237, 0.4032)	0.076
473	(0.5088, 0.4113)	0.096
498	(0.4979, 0.4136)	0.108
523	(0.4870, 0.4170)	0.121
548	(0.4766, 0.4207)	0.133
573	(0.4636, 0.4248)	0.147

Pump power-dependent

The UC intensity (I) and the pump power (P) satisfy the following relationship:[1]

$$I \propto P^n \tag{S1}$$

where n is the number of incident photon that is involved to populate the excited state from ground state.

Bandgap

The bandgap value (E_g) can be calculated based on the following equation:[2]

$$F(R) = (1 - R)^2/(2R) \tag{S2}$$

$$[F(R)hv]^{1/n} = A(hv - E_g) \tag{S3}$$

where R, hv, and A stand for reflectance coefficient, photon energy and absorption constant a, respectively. The n values of 1/2 and 2 correspond to direct and indirect

allowed transitions in the same order.

Optical thermometry

The LIR is defined by the following equation:[3]

$$LIR = Aexp\left(-\frac{\Delta E}{kT}\right) \quad \text{(S4)}$$

where A is a pre-exponential factor, depending on the radiative decay rates from the different energy states and energy state degeneracies, k is Boltzmann constant, ΔE is the energy gap between the $^2H_{11/2}$ and $^4S_{3/2}$ states and T is temperature.

The absolute sensitivity (S_a) and relative sensitivity (S_r) can be calculated using the following equations:[3]

$$S_a = \left|\frac{dLIR}{dT}\right| \quad \text{(S5)}$$

$$S_r = \left|\frac{1}{LIR}\frac{dLIR}{dT}\right| \quad \text{(S6)}$$

The temperature resolution (δT) can be determined using the following equation:[3]

$$\delta T = \frac{1}{S_r}\frac{\delta LIR}{LIR} \quad \text{(S7)}$$

where $\delta LIR/LIR$ is the uncertainty in the calculation of LIR (determined as a standard deviation in twenty measurements of LIR).

The repeatability (R) can be determined using the following equation:[3]

$$R = 1 - \frac{Max(|LIR_a - LIR_i|)}{LIR_a} \quad \text{(S8)}$$

where LIR_a and LIR_i represent the average of the LIR values and the measured LIR values (298 and 573 K) in five consecutive cycles.

The *LIR* is defined by the following equation:[3]

$$LIR = A_3T^3 + A_2T^2 + A_1T + A_0 \quad \text{(S9)}$$

where A_0, A_1, A_2 and A_3 are fitting constants of the polynomial and T is temperature.

$$S_a = \left|\frac{dLIR}{dT}\right| = 3A_3T^2 + 2A_2T + A_1 \quad \text{(S10)}$$

$$S_r = \left|\frac{1}{LIR}\frac{dLIR}{dT}\right| = \frac{1}{LIR}(3A_3T^2 + 2A_2T + A_1) \quad \text{(S11)}$$

The CIEy is defined by the following equation:[4]

$$CIEy = Aexp\left(-\frac{B}{T}\right) + C \quad \text{(S12)}$$

where A, B, and C are fitting constants and T is temperature.

Chromaticity shift

The chromaticity shift (ΔE_s) is defined by the following equation:[5]

$$\Delta E_s = \sqrt{(u_f' - u_i')^2 + (v_f' - v_i')^2 + (w_f' - w_i')^2} \quad \text{(S13)}$$

where $u' = 4x/(3 - 2x + 12y)$, $v' = 9y/(3 - 2x + 12y)$, and $w' = 1 - u' - v'$. u' and v' are the chromaticity coordinates in the $u'v'$ uniform color space. x and y are the chromaticity coordinates in the CIE1931 color space. i and f represent room temperature and working temperature, respectively.

References

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[3] J. Y. Chen, J. Q. Chen, L. J. Li, W. N. Zhang, L. P. Chen, H. Guo, A four-mode high-sensitive optical thermometer based on $Ca_3LiZnV_3O_{12}$:Sm^{3+} phosphors, Mater.

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