

Supplementary Information

Superlattice-stabilized structure and charge transfer assisted photoluminescence enhancement in a samarium-doped high entropy perovskite oxide

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Table S.1 Crystal structural parameters from Rietveld powder XRD refinement for $\text{Ca}_{0.98}\text{Sm}_{0.02}(\text{M}_5)\text{O}_3$ and $\text{Ca}_{0.98}\text{Sm}_{0.02}\text{SnO}_3$.

	$\text{Ca}_{0.98}\text{Sm}_{0.02}(\text{M}_5)\text{O}_3$	$\text{Ca}_{0.98}\text{Sm}_{0.02}\text{SnO}_3$
Lattice parameters (Å)		
a	5.5140	5.5318
b	7.8816	7.9061
c	5.6634	5.6801
Bond length (Å)		
B-O ₁	2.000	2.055
B-O ₂₁	2.014	2.057
B-O ₂₂	2.071	2.056
B-O ₂₃	2.014	2.057
B-O ₂₄	2.071	2.056
Bond angle (°)		
O1-B-O21	86.5565	89.9905
O1-B-O22	93.4435	90.0095
O1-B-O23	91.3169	88.3347
O1-B-O24	88.6804	91.6653

Table S.2 The Raman bands position of Sm³⁺-doped phosphor samples.

	Ca(M ₅)O ₃	CaSnO ₃ [1]	CaZrO ₃ [2]	CaHfO ₃	CaTiO ₃ [3]	
O-B-O bending modes	189	167	147	151	159	
		187	191		184	
	235		216	214	228	
				233		
	258		265	265	250	
	286	282	289	293	290	
	353	361	360	362	340	
			389			
	B-O ₃ torsional modes	452	447	441	450	
		480		472	480	473
					498	
B-O symmetric stretching	525		549	588	634	

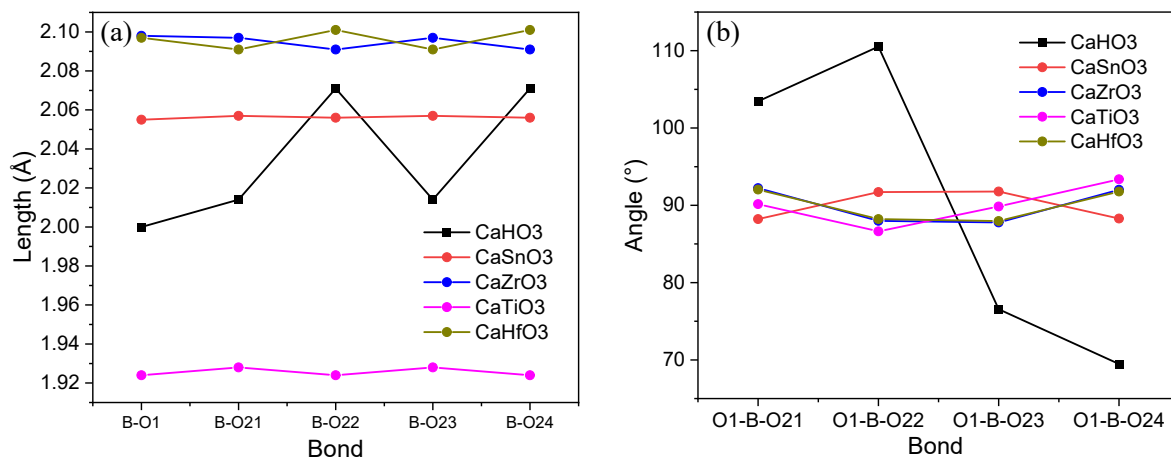


Figure S1. Bond length (a) and angle (b) fluctuations for all the compositions.

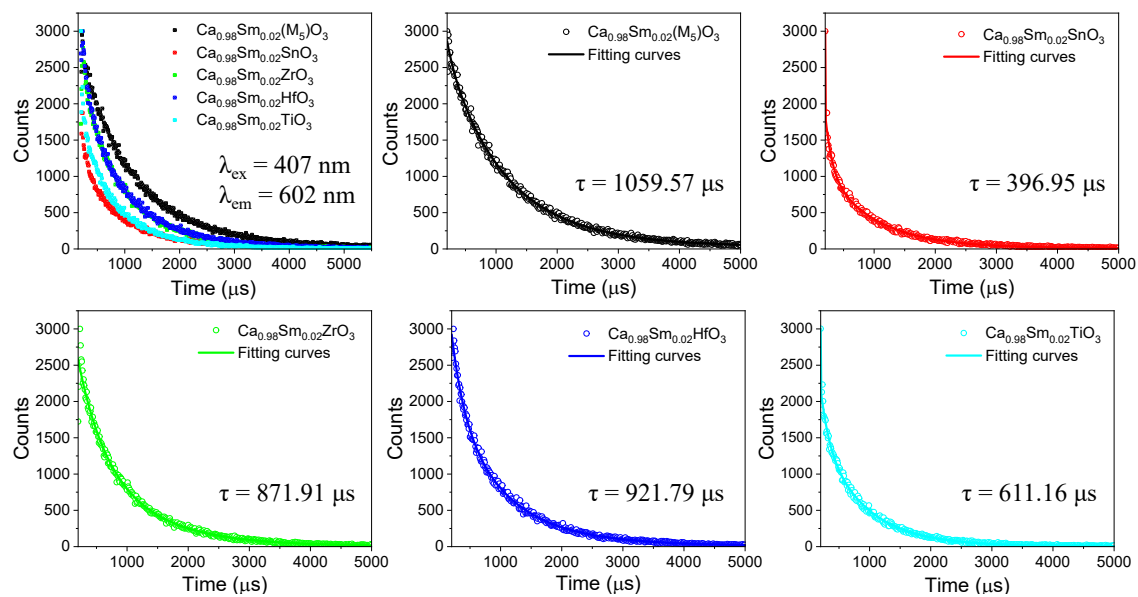


Figure S2. The PL lifetime curve and after fitting of Sm^{3+} -doped phosphor samples under 407 nm excitation.

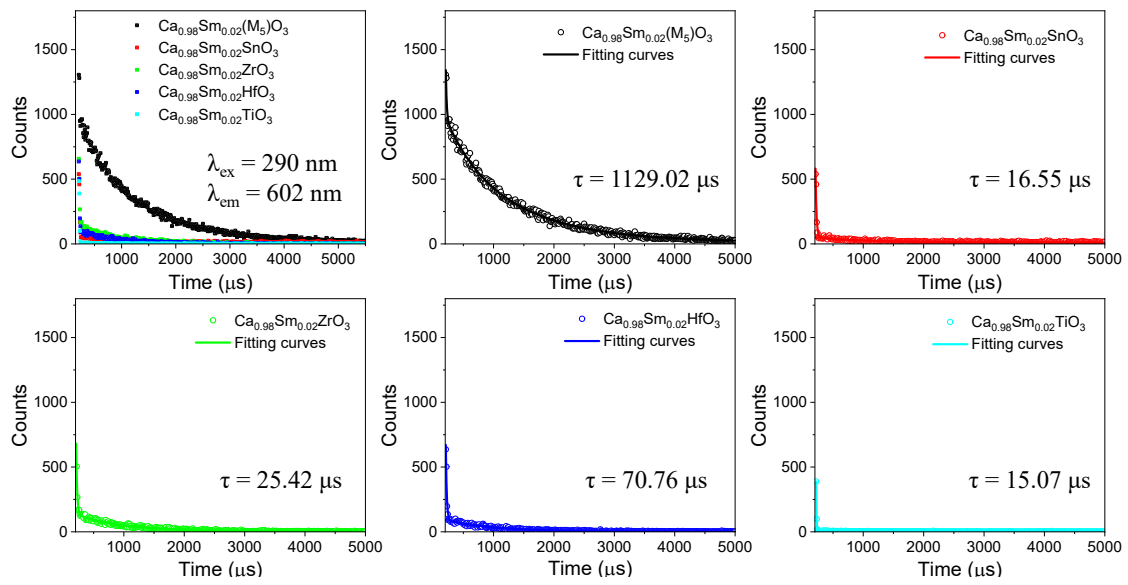


Figure S3. The PL lifetime curve and after fitting of Sm^{3+} -doped phosphor samples under 290 nm excitation.

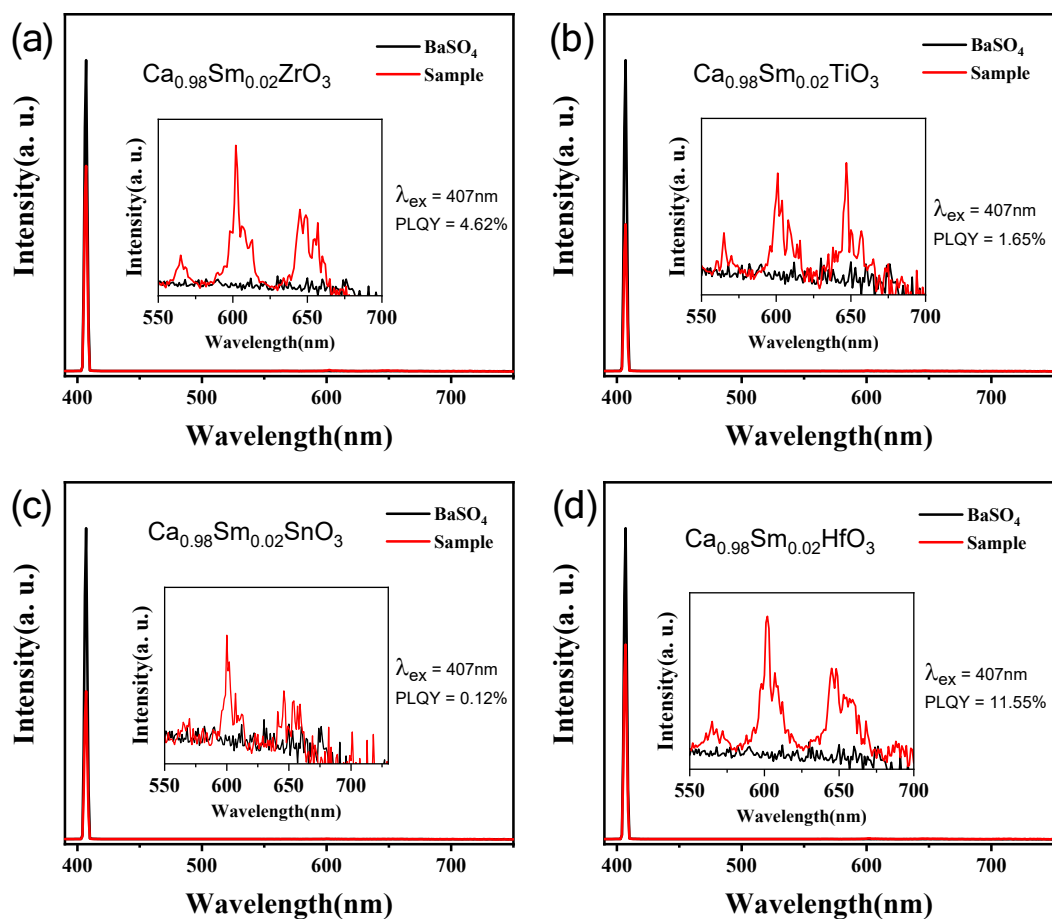


Figure S4. The PLQY measurement of Ca_{0.98}Sm_{0.02}ZrO₃ (a), Ca_{0.98}Sm_{0.02}TiO₃ (b), Ca_{0.98}Sm_{0.02}SnO₃ (c) and Ca_{0.98}Sm_{0.02}NbO₃ (d) phosphor.

Decay lifetime

The optical decay time is fitted via the third-order exponential function with the following equation [4]:

$$I(t) = I_0 + A_1 \exp(-t/\tau_1) + A_2 \exp(-t/\tau_2) + A_3 \exp(-t/\tau_3) \quad (S1)$$

Where t represents the time, $I(t)$ is the emission intensity corresponding to time t , I_0 is the initial emission intensity corresponding to time $t = 0$, A_1 , A_2 and A_3 are constants, τ_1 , τ_2 and τ_3 are lifetimes for the exponential components. The average lifetime τ can be obtained by the formula as follows:

$$\tau = (A_1\tau_1^2 + A_2\tau_2^2 + A_3\tau_3^2) / (A_1\tau_1 + A_2\tau_2 + A_3\tau_3) \quad (S2)$$

Color coordinates

The quality of the color produced by Sm^{3+} -doped $\text{Ca}(\text{M}_5)\text{O}_3$ is evaluated by calculating chromaticity Commission International de l'Eclairage (CIE1931) coordinates. The calculations are based on the evaluation of three CIE coordinates x , y and z defined by the equation [5]:

$$\begin{cases} x = X/(X + Y + Z) \\ y = Y/(X + Y + Z) \\ z = Z/(X + Y + Z) \end{cases} \quad (S3)$$

Where $x + y + z = 1$, and depends upon the tristimulus values, X , Y and Z . However, to specify the chromaticity of a sample, two independent variables x and y , are generally used. The values for X , Y and Z are proportional to the spectral intensity of the material, $I(\lambda)$, and chromatic functions of the observer, \bar{x} , \bar{y} and \bar{z} as the following equation:

$$\begin{cases} X = \int_{450nm}^{750nm} I(\lambda) \cdot \bar{x}(\lambda) d\lambda \\ Y = \int_{450nm}^{750nm} I(\lambda) \cdot \bar{y}(\lambda) d\lambda \\ Z = \int_{450nm}^{750nm} I(\lambda) \cdot \bar{z}(\lambda) d\lambda \end{cases} \quad (S4)$$

Correlated color temperature (CCT)

The parameter of CCT can be speculated using McCamy empirical formula, which is illustrated as [6]:

$$CCT = -449n^3 + 3525n^2 + 6823.3n + 5520.33 \quad (S5)$$

Where $n = (x - 0.3320)/(y - 0.1858)$.

Color purity [7]

The parameter of color purity [7] can be obtained via the follow equation [8]:

$$CP = \sqrt{(x - x_i)^2 + (y - y_i)^2} / \sqrt{(x_d - x_i)^2 + (y_d - y_i)^2} \quad (S6)$$

Where (x_i, y_i) is the illuminant point (0.3101, 0.3162), which corresponds to the CIE1931 Standard Source C. The color coordinates (x_d, y_d) come from the domain emission.

PL quantum efficiency

PL quantum efficiency (PLQY) can be calculated according to the formula as follows [5]:

$$PLQY = \int L_S / \left(\int E_R - \int E_S \right) \quad (S7)$$

Where L_S is the emission spectrum of the sample, E_R and E_S stand for the excitation spectra without and with the sample in the integrating sphere, respectively.

Thermal quenching mechanism

To investigate the thermal quenching mechanism of the Sm^{3+} -doped $\text{Ca}(\text{M}_5)\text{O}_3$ sample, the activation energy [3] was calculated via the following Arrhenius equation [9]:

$$\ln[(I_0/I(T))-1] = \ln A - (E_a/kT) \quad (S8)$$

Where I_0 is the initial emission intensity of the phosphor at room temperature, $I(T)$ is the emission intensity at testing temperature T , A is an invariable constant for a certain host, and k represent the Boltzmann constant ($8.629 * 10^{-5}$ eV/K). on the basis of the equation, the relationship between $\ln[(I_0/I(T))-1]$ versus $1/kT$ is shown.

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