Luminescence Properties and Judd-Ofelt Analysis of Tb^{3+} Doped Sr_2YTaO_6 Double Perovskite Phosphors for White LED Applications

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Support Information

1. J-O calculation process based on emission spectra and radiative transition lifetime

The relative integrated PL intensity for $^5D_4 \rightarrow {}^7F_J$ of Tb^{3+} ions can be firstly calculated from the PL spectrum of SYT: 5 mol% Tb^{3+} phosphor. Meanwhile, the sum of relative integrated PL intensity of $^5D_4$ energy level of Tb^{3+} ions ($I = \sum_{J=0-6} I_{7_{F_J}}$) is usually proportional to the total radiative transition rate $\sum_{J=0-6} A_{7_{F_J}}$ [1] [2], and the relationship can be represented as follows:

$$I = a \sum_{J=0-6} A_{7_{F_J}} \quad \text{(S1)}$$

where $\sum_{J=0-6} A_{7_{F_J}}$ is equal to the reciprocal of the radiative transition lifetime τ_0, and the expression is written as

$$\sum_{J=0-6} A_{7_{F_J}} = \frac{1}{\tau_0} \quad \text{(S2)}$$

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According to the above analysis, substitute τ_0 = 3.63 ms into Eq. (S2) and combine it with Eq. (S1), the coefficient a can be confirmed as 9.74×10^{-4}. And then, the radiative transition rate from $^5D_4$ to ^7F_J were gotten by using Eq. (S3).

$$I_{^7F_J} = a \times A_{^7F_J} \tag{S3}$$

Furthermore, the radiative transition rates for a certain transition from state J to state J′ can be expressed as

$$A^{md}_{J-J'} = \frac{64\pi^4 v^3}{3h(2J+1)} n^3 \left(\frac{eh}{4\pi m_e c}\right)^2 \langle \Psi J \| L + 2S \| \Psi' J' \rangle^2 \tag{S4}$$

$$A^{ed}_{J-J'} = \frac{64\pi^4 e^2 v^3}{3h(2J+1)} \frac{n(n^2+2)^2}{9} \sum_{\lambda=2,4,6} \Omega_\lambda \langle \Psi J \| U^{(\lambda)} \| \Psi' J' \rangle^2 \tag{S5}$$

where A^{md} and A^{ed} are the contribution from magnetic dipole (MD) to the transition rate and the contribution from electric dipole (ED), respectively. v is the central wavenumber for J→J′ transition. h is Planck's constant ($h = 6.626\times10^{27}$ erg·s), 2J+1 is the degeneracy of the initial state, n is the refractive index of the host (here n is 1.98 for SYT host), and $\langle \Psi J \| L + 2S \| \Psi' J' \rangle^2$ is the squared matrix element for MD line strength.[3] e is the charge of an electron ($e = 4.80\times10^{-10}$ esu) and $\langle \Psi J \| U^{(\lambda)} \| \Psi' J' \rangle$ is the reduced matrix element for the J→J′ transition.[3] Based on the above analysis, by applying the least squares method to the equations corresponding to all the transitions from $^5D_4$ to ^7F_J, the parameters Ω_λ (λ = 2, 4, 6) were calculated.

Additionally, the fluorescence branch ratios for the $^5D_4$ energy level under 318 nm excitation can be derived from the following equation:

$$\beta = \frac{A_{J-J'}}{\sum_{J=0-6} A_{J-J'}} \tag{S6}$$

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[2] Tian, Y.; Chen, B.; Hua, R.; Sun, J.; Cheng, L.; Zhong, H., et al., Optical transition, electron-phonon coupling and fluorescent quenching of $La_2(MoO_4)_3:Eu^{3+}$ phosphor. *J Appl Phys* **2011**, *109* (5), 053511.

[3] Loiko, P.; Mateos, X.; Dunina, E.; Kornienko, A.; Volokitina, A.; Vilejshikova, E., et al., Judd-Ofelt modelling and stimulated-emission cross-sections for Tb^{3+} ions in monoclinic $KYb(WO_4)_2$ crystal. *J Lumin* **2017**, *190*, 37-44.

2. Calculation for CCT and CRI

Based on the obtained color coordinates, the CCT value can be calculated by using the McCamy's approximate[1]

$$CCT = -437n^3 + 3601n^2 - 6861n + 5514.31 \quad \text{(S7)}$$

where $n = \frac{x - x_e}{y - y_e}$. (x, y) is the chromaticity coordinates. (x_e, y_e) is the coordinate of the epicenter and its value is (0.332, 0.186).

Moreover, general color rending index (CRI) is the average of eight special color rending indices.[2]

$$CRI = \frac{1}{8}\sum_{i=1}^{8} R_i = \frac{1}{8}\sum_{i=1}^{8}(100 - 4.6\Delta E_i) \quad \text{(S8)}$$

where R_i is the special color rendering index of a certain color sample *i*, ΔE_i is the corresponding color difference between the sample under the reference light source and the test light source.

[1] McCamy, C. S., Correlated color temperature as an explicit function of chromaticity coordinates. *Color Res Appl* **1992**, *17* (2), 142-144.

[2] Jin, X.; Xie, Y.; Tang, R.; Geng, X.; Che, J.; Lou, L., et al., Novel double perovskite Sr_3WO_6: Sm^{3+}, Na^+ orange-red emitting phosphors with high thermal stability for white LEDs. *J Alloy Compd* **2022**, *899*, 162739.