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

Li Wang[1, 2], Yuhang Zhang[1, *], Duan Gao[1], Xuezhu Sha[1], Xin Chen[1], Yanqiu Zhang[1], Jinsu Zhang[1], Xizhen Zhang[1], Yongze Cao[1], Yichao Wang[1], Xiangping Li[1], Sai Xu[1], Hongquan Yu[1], Baojiu Chen[1, *]

1 School of Science, Dalian Maritime University, Dalian, 116026, Liaoning, PR China
2 College of Medical Laboratory, Dalian Medical University, Dalian, 116044, Liaoning, PR China

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

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

* Corresponding Authors: YHZhang email: yuhangzhang@dlmu.edu.cn; BJChen email: bjchen@dlmu.edu.cn
Fax and Tel.: 86-411-8472-8909

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).

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

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:

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

［1］ Tian, B.; Chen, B.; Tian, Y.; Li, X.; Zhang, J.; Sun, J., et al., Excitation pathway and temperature dependent luminescence in color tunable $Ba_5Gd_8Zn_4O_{21}:Eu^{3+}$ phosphors. *J Mater Chem C* **2013**, *1* (12), 2338.

［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.

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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]

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

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.