Supporting Information

High-performance dual-mode self-calibrating optical thermometry for Er³⁺, Li⁺ co-doped oxides

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Structure and characteristics

The unit cell structure of the yttrium oxide (Y_2O_3) is visualized based on the #155173 of the ICSD (Inorganic Crystal Structure Database)¹. As presented in Figure S1(a), Y_2O_3 crystallized in cubic structure ($\alpha=\beta=\gamma=90$) with the Ia-3 space group, with the lattice parameters of a= 10.6039 (1) Å, b = 10.6039 (1) Å, c = 10.6039 (1) Å, and V= 1192.33 Å³. The Y³⁺ atoms at two different Wyckoff position form octahedral coordination with each of the six oxygen atoms. Here, 24 identical Y_dO₆ octahedrons have Y-O bond lengths ranging from 2.256 to 2.34 Å, while the Y-O bond lengths of Y_bO₆ octahedrons at 8 different positions are all 2.29 Å. Besides, the close ionic radii of Er³⁺ (~0.89 Å)² as compared with Yb³⁺ (~0.9 Å)³ facilitates the replacement of Y³⁺ upon doping with Er³⁺. While the Li⁺ (~0.59 Å)³ ions with a smaller radius are more likely to enter into interstitial sites (Figure S1(b)).



Figure S1. a) Crystal structure of the Y_2O_3 (red and gray-white spheres are oxygen and yttrium atoms, respectively). b) Possible crystal structure of Er, Li co-doped Y_2O_3 .

The normalized XRD patterns of Y_2O_3 : $Er^{3+}10\%$, Li^+y (y=0, 1, 3, 5, 7, 10 and 15 mol%) phosphor powders are shown in Figure S2(a). All the XRD peaks agree well with the data of the standard pattern (JCPDS NO.79-1257), indicating that the synthesized sample has a pure phase structure without any secondary phase. In addition, all the diffraction peaks are significantly enhanced with the increase of Li^+ doping concentration, implying a remarkable improvement in crystallinity. In addition, as shown in Figure S2(b), the main diffraction peak is slightly shifted to the left based on Y_2O_3 : $Er^{3+}10\%$, which is due to lattice expansion caused by interstitial doping of the Li^+ ions. However, the right shift phenomenon at $Li^+15\%$ should be the replacement of the Y^{3+} ions by Li^+ after interstitial doping saturation.



Figure S2. a) Normalized XRD patterns of Y_2O_3 : $Er^{3+}10\%$, Li^+y (*y*=0, 1, 3, 5, 7, 10 and 15 mol%) samples and standard pattern of the Y_2O_3 (JCPDS NO.79-1257) (The

amplified XRD pattern is shown in Figure S2(b)).



Figure S3. UC spectra of Y_2O_3 : 10%Er³⁺, 10%Li⁺ phosphors at different temperatures (123-443 K).



Figure S4. Relative sensitivity (S_R) and absolute sensitivity (S_A) values of Y_2O_3 : 10%Er³⁺, phosphor in the temperature range of 303-443 K.

Reference

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