Supporting Information

Dye Encapsulated Terbium-Based Metal-Organic Framework for Ratiometric Temperature Sensing

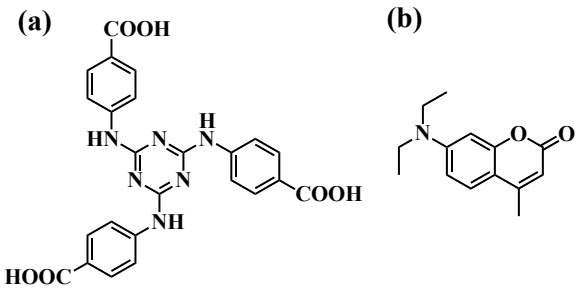
Tifeng Xia, Tao Song, Yuanjing Cui,* Yu Yang and Guodong Qian*

State Key Laboratory of Silicon Materials, Cyrus Tang Center for Sensor Materials and Applications, School of Materials Science & Engineering, Zhejiang University, Hangzhou 310027, China

*Corresponding authors:

Yuanjing Cui: cuiyj@zju.edu.cn

Guodong Qian: gdqian@zju.edu.cn.



Scheme S1 Structure of (a) 4,4',4"-s-triazine-1,3,5-triyltri-*p*-aminobenzoic acid (H_3TATAB) and (b) 7-diethylamino-4-methylcoumarin (C460).

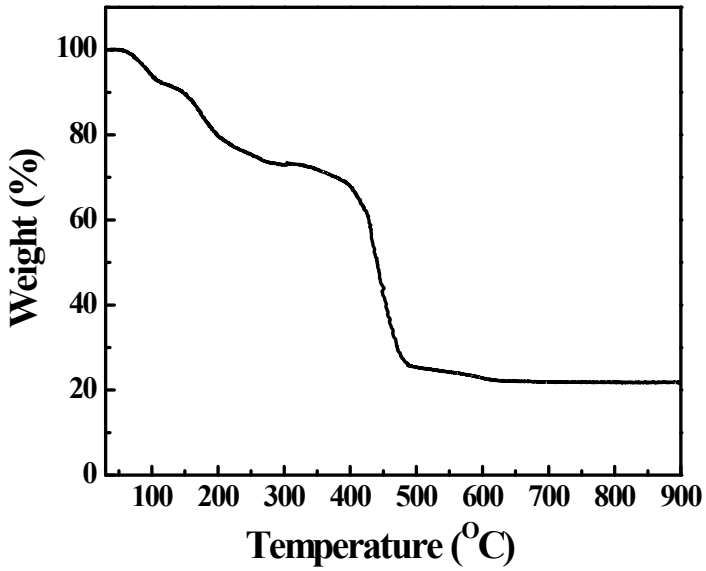


Fig. S1 The TGA curves of **TbTATAB**.

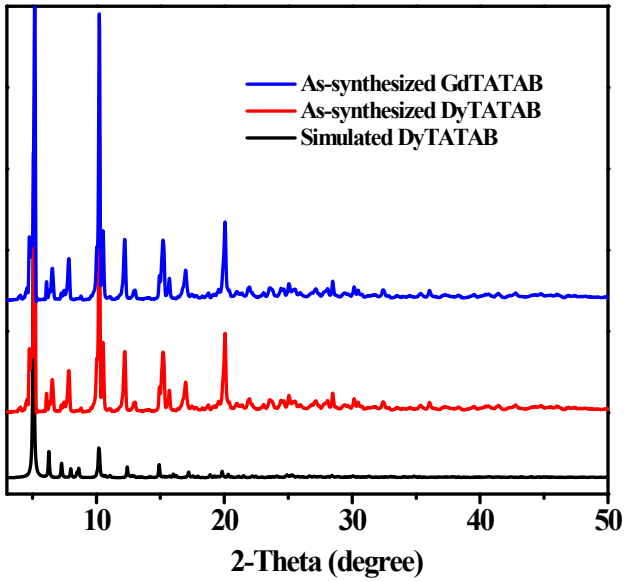


Fig. S2 PXRD patterns of as-synthesized **DyTATAB** and **GdTATAB.**

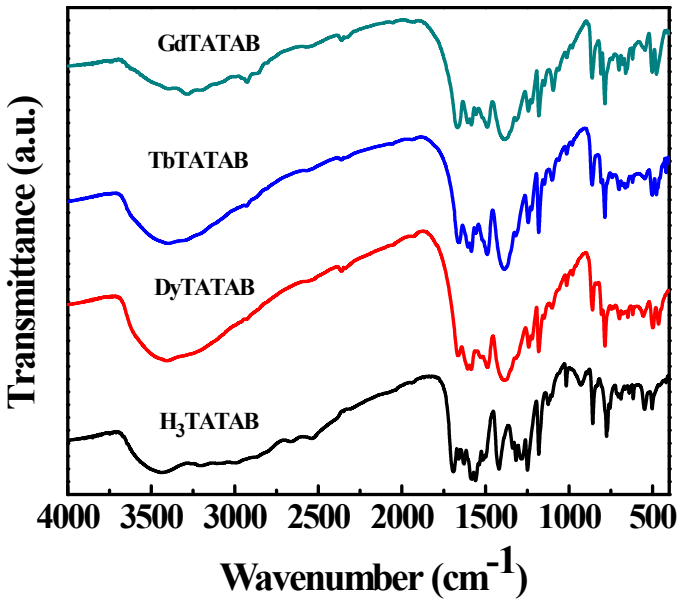


Fig. S3 FT-IR spectra of H_3TATAB and **LnTATAB** (Ln = Dy, Tb, and Gd).

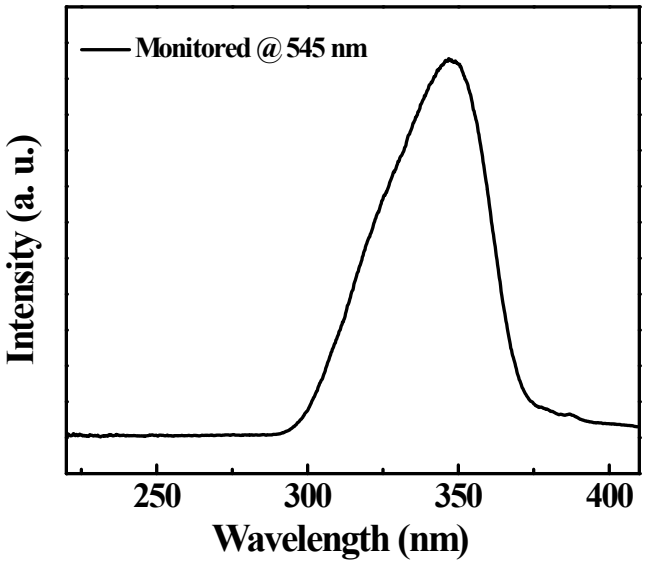


Fig. S4 Excitation spectra of **TbTATAB** monitored at 545 nm.

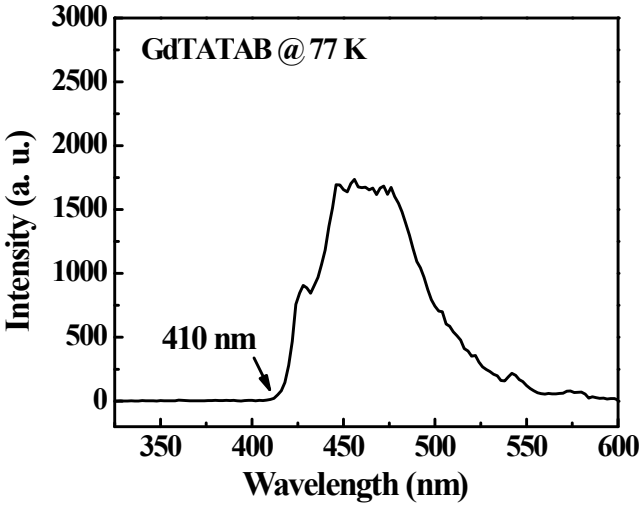


Fig. S5 Phosphorescence spectra of **GdTATAB** at 77 K.

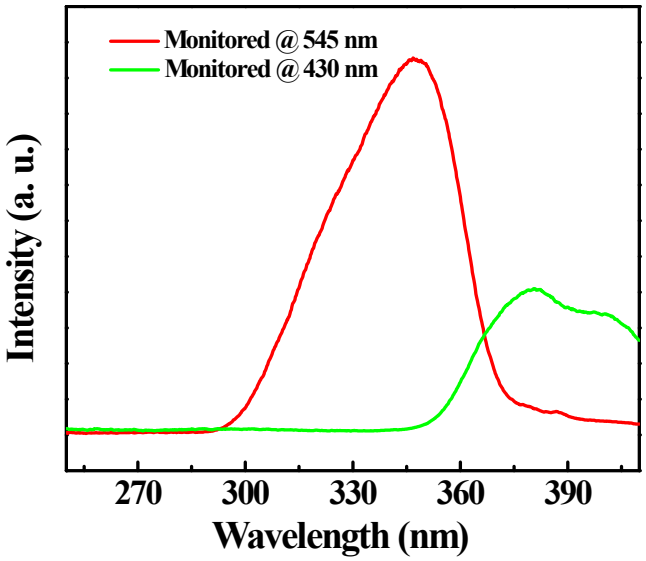


Fig. S6 Excitation spectra of **TbTATAB⊃C460** monitored at 430 nm and 545 nm, respectively.

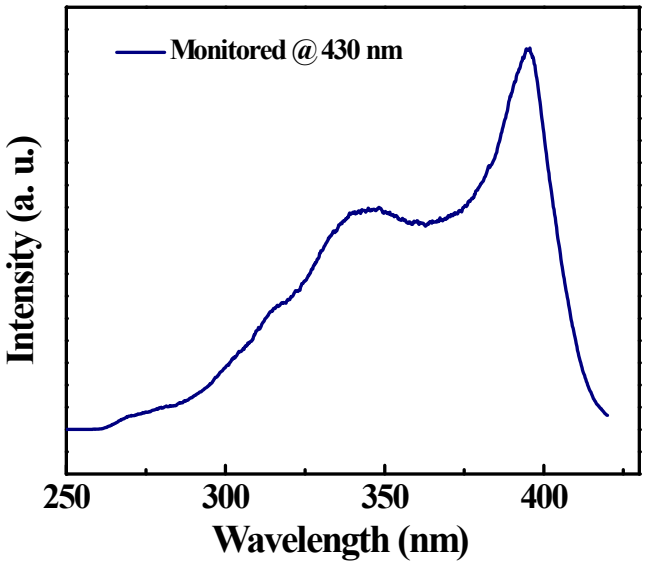


Fig. S7 Excitation spectra of C460 monitored at 430 nm.

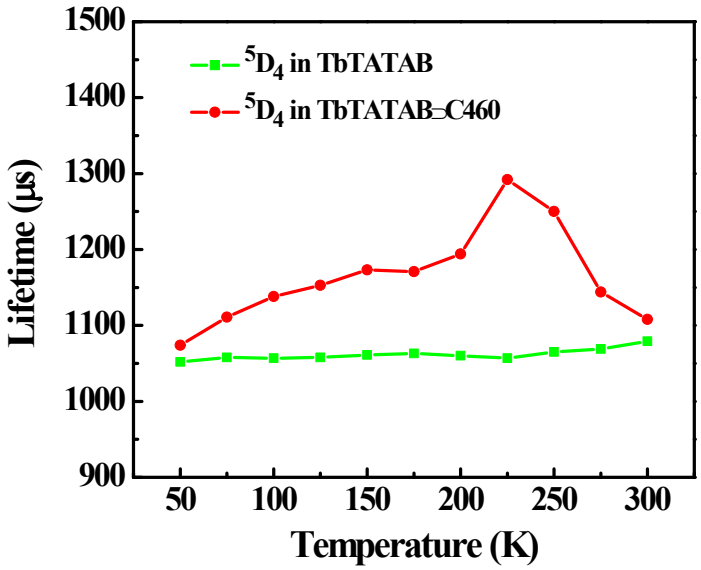


Fig. S8 Temperature-dependent lifetime of $^5D_4$ in **TbTATAB** and **TbTATAB⊃C460**.

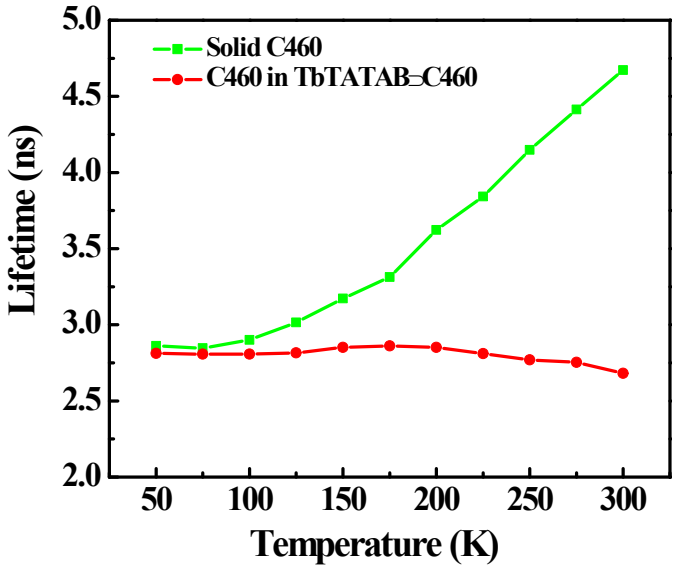


Fig. S9 Temperature-dependent lifetime of C460 at 430 nm in solid C460 and **TbTATAB⊃C460**.

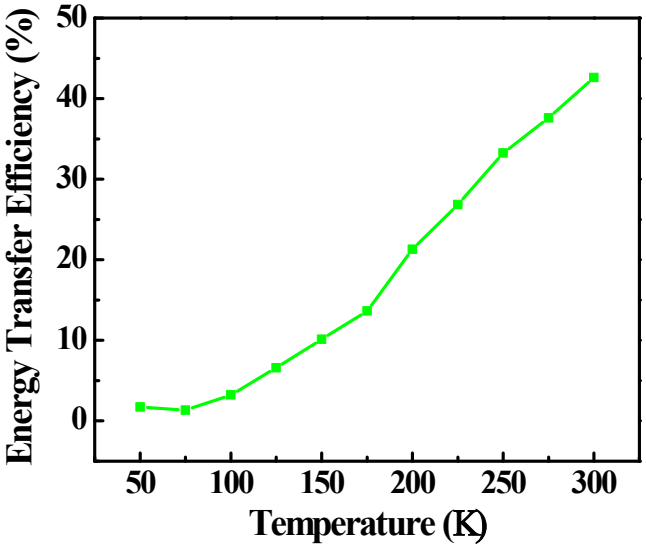


Fig. S10 Temperature-dependent energy transfer efficiency of **TbTATAB⊃C460**.

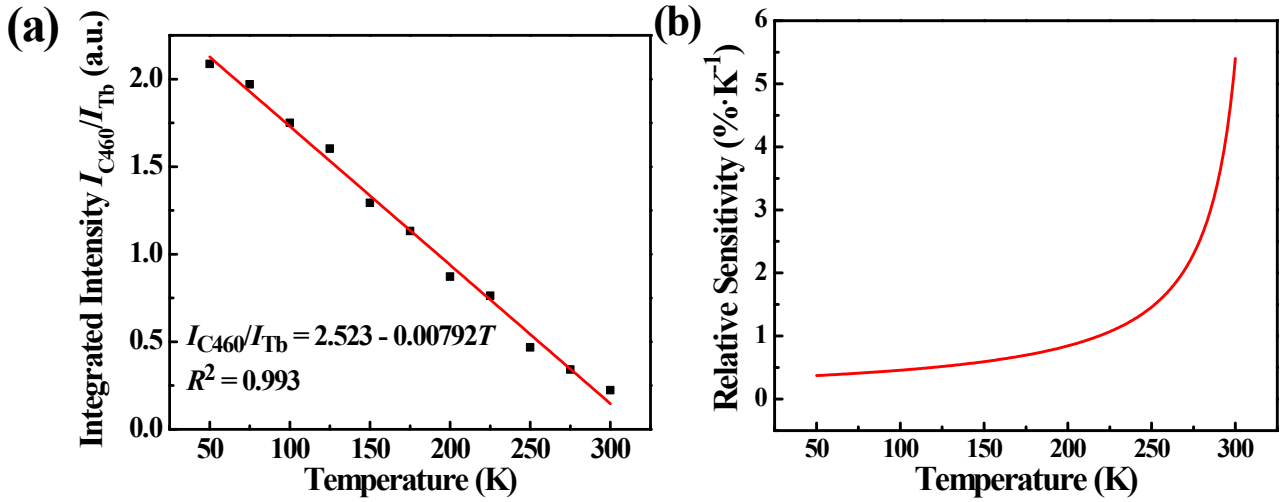


Fig. S11 (a) Temperature-dependent integrated intensity ratio of C460 (385-480 nm) to Tb^{3+} (535-560 nm) and the fitted curve for **TbTATAB⊃C460**. (b) Temperature-dependent relative sensitivity (S_r) of **TbTATAB⊃C460**.

The calculation method of the amount of C460 in MOFs

Luminescent intensities of different concentration of C460 in DMF solution were measured and repeated five times, and then the average values were calculated. Therefore, the relationship (Equation S1) for the intensity-concentration of C460 in DMF solution could be obtained. Crystals (about 22 mg) of three different **TbTATAB⊃C460** composites were dissolved in 5 mL DMF solution containing 20 μL HCl (12 mol L^{-1}) to become clear solution. The resulting solution was diluted 10 times with DMF. The luminescent intensity of the solution was measured, and the concentration was calculated through Equation S1.

$$y = 28.33 + 5.2 \times 10^{6} x \qquad \text{(S1)}$$

y—luminescent intensity;

x—concentration;

then the contents of C460 in two different **TbTATAB⊃C460** composites were calculated to be 3.67% and 8.23% mg mg^{-1}, respectively.

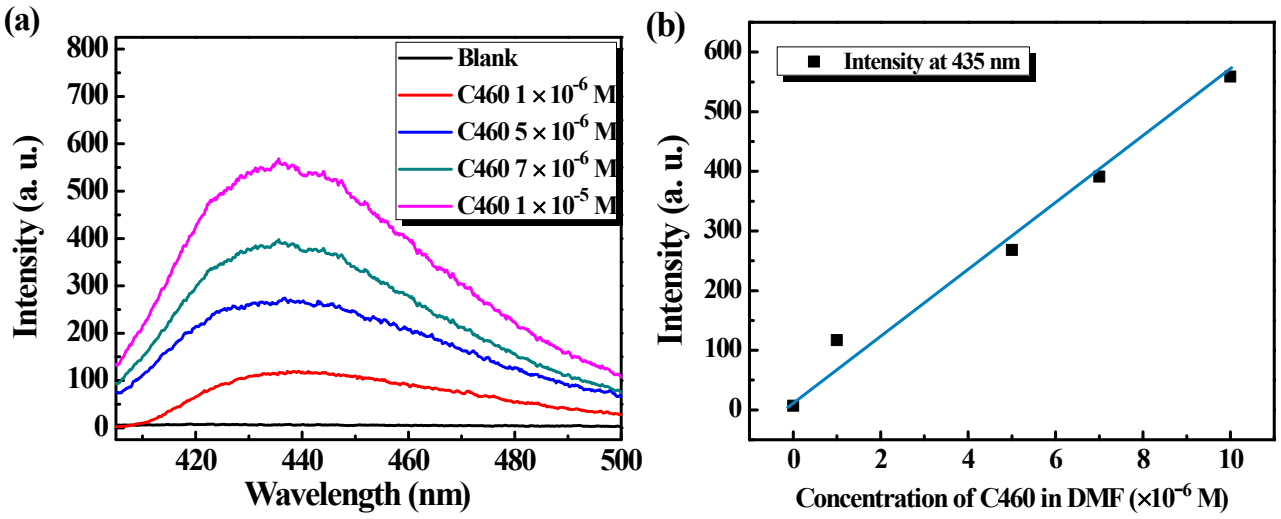


Fig. S12 (a) The intensity of C460 in DMF with different concentrations and (b) the fitted curve between the intensity and the concentration.

Table S1. Crystallographic data collection and refinement result for **DyTATAB.**

Compound	**DyTATAB**
CCDC No.	1439404
Chemical formula	$C_{48}H_{24}Dy_2N_{12}O_{15}$
Formula weight	1333.79
Temperature (K)	296
Wavelength (Å)	0.71073
Crystal system	monoclinic
Space group	$P\,2_1/c$
a (Å)	29.162(4)
b (Å)	21.924(2)
c (Å)	14.955(2)
α (°)	90
β (°)	103.380(7)
γ (°)	90

Volume (Å^3)	9302(2)
Z	4
Absorbance coefficient (mm^{-1})	1.638
absorption correction T_{max}	0.0046
absorption correction T_{min}	0.0002
F(000)	2592
Crystal size (mm^3)	0.45×0.15×0.12
R_{int}	0.0720
$R1$, $wR2$ ($I>2\sigma(I)$[a]	0.1216, 0.3292
$R1$, $wR2$ (all data)[a]	0.1335, 0.3669
goodness of fit on F^2	0.986

[a] $R1 = \sum\left(|F_o| - |F_c|\right)/\sum|F_o|; wR2 = \left[\frac{\sum w\left(|F_o| - |F_c|^2\right)}{\sum wF_o^2}\right]^{1/2}$