materials

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*Supplementary Materials*

# Narrow-Band Deep-Blue Emission and Superior Thermal Stability of Fluoroaluminate Phosphor based on Tungsten Bronze-Type Mineral Structure

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**Table S1.** The refinement results of the atomic positions and site occupancies of TB-type KCAF:0.005$Eu^{2+}$ and KCAF:0.013$Eu^{2+}$ phosphors.

| KCAF:0.005$Eu^{2+}$ | | | | | KCAF:0.013$Eu^{2+}$ | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **x** | **y** | **z** | **occupancy** | **Atom** | **x** | **y** | z | occupancy |
| K1 | 0.0094 | 0.0000 | 0.0000 | 1.0000 | K1 | 0.0094 | 0.0000 | 0.0000 | 1.0000 |
| K2 | −0.0218 | 0.0143 | 0.1667 | 1.0000 | K2 | −0.0218 | 0.0143 | 0.1667 | 1.0000 |
| Ca1 | 0.2443 | 0.0258 | 0.0834 | 0.9970 | Ca1 | 0.2443 | 0.0258 | 0.0834 | 0.9910 |
| Ca2 | 0.0000 | 0.5201 | 0.2500 | 0.9980 | Ca2 | 0.0000 | 0.5201 | 0.2500 | 0.9960 |
| Al1 | −0.0080 | 0.4991 | 0.0799 | 1.0000 | Al1 | −0.0080 | 0.4991 | 0.0799 | 1.0000 |
| Al2 | 0.2398 | 0.2428 | −0.0864 | 1.0000 | Al2 | 0.2398 | 0.2428 | −0.0864 | 1.0000 |
| Al3 | 0.2481 | 0.7696 | 0.2468 | 1.0000 | Al3 | 0.2481 | 0.7696 | 0.2468 | 1.0000 |
| F1 | 0.2092 | 0.7848 | 0.0106 | 1.0000 | F1 | 0.2092 | 0.7848 | 0.0106 | 1.0000 |
| F2 | −0.0289 | 0.5124 | 0.1558 | 1.0000 | F2 | −0.0289 | 0.5124 | 0.1558 | 1.0000 |
| F3 | 0.5132 | 0.0000 | 0.0000 | 1.0000 | F3 | 0.5132 | 0.0000 | 0.0000 | 1.0000 |
| F4 | 0.2713 | 0.7326 | 0.1669 | 1.0000 | F4 | 0.2713 | 0.7326 | 0.1669 | 1.0000 |
| F5 | 0.2751 | 0.3134 | 0.1773 | 1.0000 | F5 | 0.2751 | 0.3134 | 0.1773 | 1.0000 |
| F6 | 0.0539 | 0.2796 | 0.0841 | 1.0000 | F6 | 0.0539 | 0.2796 | 0.0841 | 1.0000 |
| F7 | −0.0675 | 0.2725 | −0.0702 | 1.0000 | F7 | −0.0675 | 0.2725 | −0.0702 | 1.0000 |
| F8 | 0.8902 | 0.2464 | 0.2574 | 1.0000 | F8 | 0.8902 | 0.2464 | 0.2574 | 1.0000 |
| F9 | 0.8914 | 0.7792 | 0.2681 | 1.0000 | F9 | 0.8914 | 0.7792 | 0.2681 | 1.0000 |
| F10 | 0.1262 | 0.6017 | 0.0939 | 1.0000 | F10 | 0.1262 | 0.6017 | 0.0939 | 1.0000 |
| F11 | 0.1421 | 0.4030 | 0.4284 | 1.0000 | F11 | 0.1421 | 0.4030 | 0.4284 | 1.0000 |
| F12 | 0.1660 | −0.0402 | 0.1034 | 1.0000 | F12 | 0.1660 | −0.0402 | 0.1034 | 1.0000 |
| F13 | 0.1805 | 0.0540 | 0.4269 | 1.0000 | F13 | 0.1805 | 0.0540 | 0.4269 | 1.0000 |
| F14 | 0.2318 | 0.5180 | 0.2617 | 1.0000 | F14 | 0.2318 | 0.5180 | 0.2617 | 1.0000 |
| Eu1 | 0.2443 | 0.0258 | 0.0834 | 0.0030 | Eu1 | 0.2443 | 0.0258 | 0.0834 | 0.0090 |
| Eu2 | 0.0000 | 0.5201 | 0.2500 | 0.0020 | Eu2 | 0.0000 | 0.5201 | 0.2500 | 0.0040 |

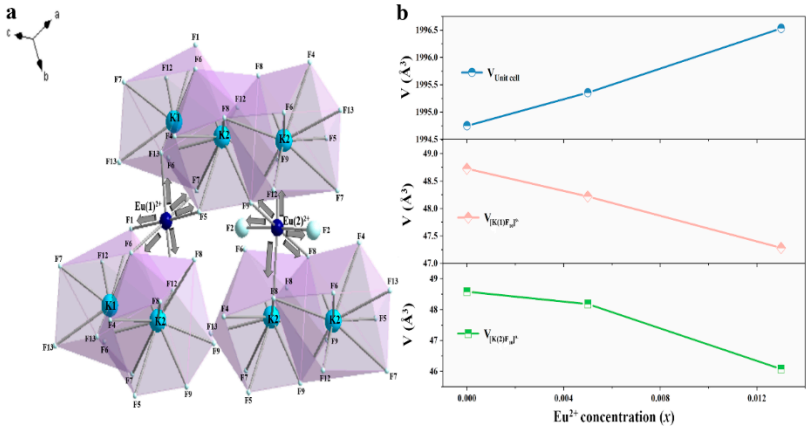



**Figure S1. (a)** The coordination environments of $K^+$ and $Eu^{2+}$ cations in the KCAF host lattice. **(b)** Changes of the volume for unit cell, $[K(1)F_{10}]^{9-}$, and $[K(2)F_{10}]^{9-}$ polyhedrons.

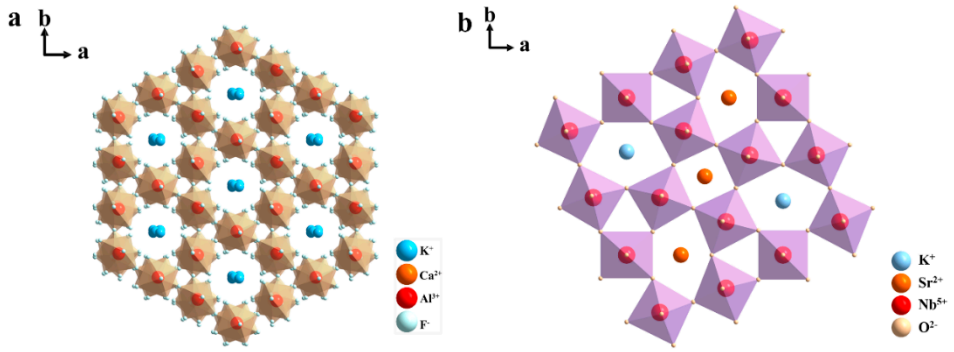



**Figure S2.** Crystal structure of **(a)** KCAF and **(b)** $Sr_2KNb_5O_{15}$ hosts from the [001] direction.

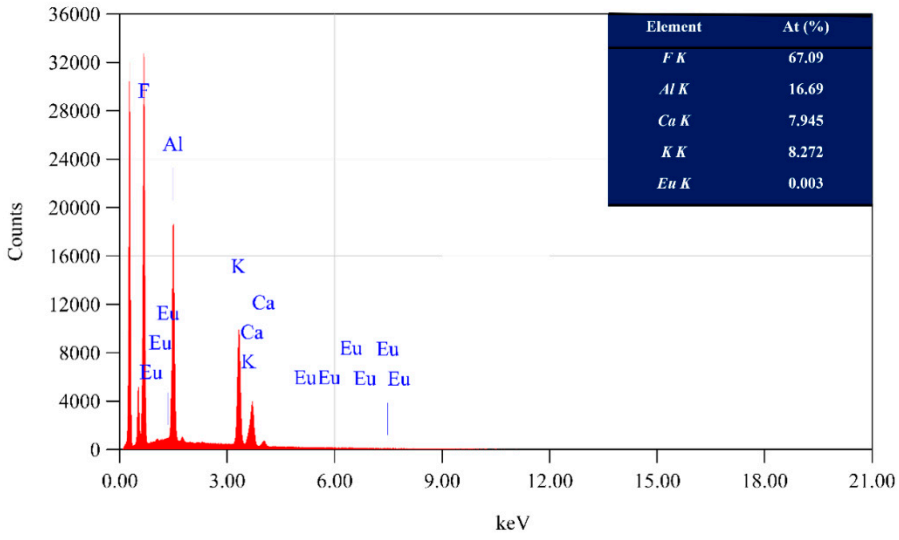



**Figure S3.** Energy-dispersive spectrum of KCAF:0.005$Eu^{2+}$ phosphor, and the inset is the respective atom percentage of KCAF:0.005$Eu^{2+}$.

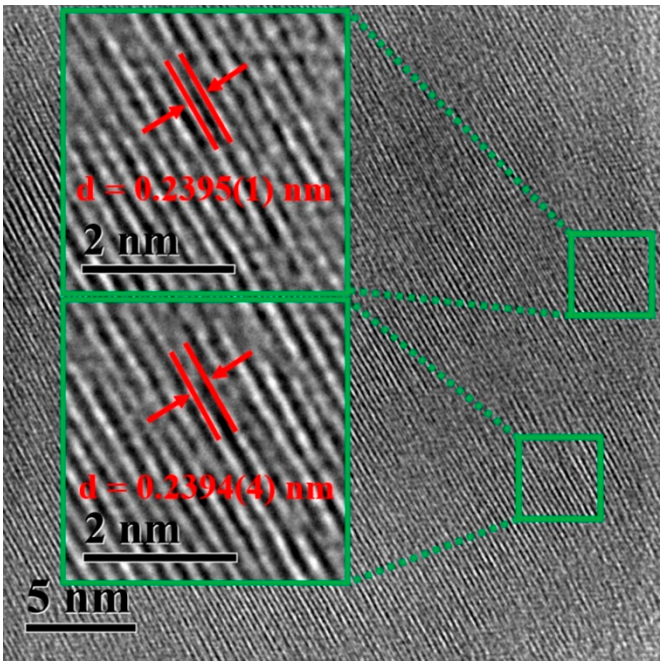



**Figure S4.** High-resolution TEM image of KCAF:0.005$Eu^{2+}$. The insets are the selected magnification areas in the corresponding high-resolution TEM image.

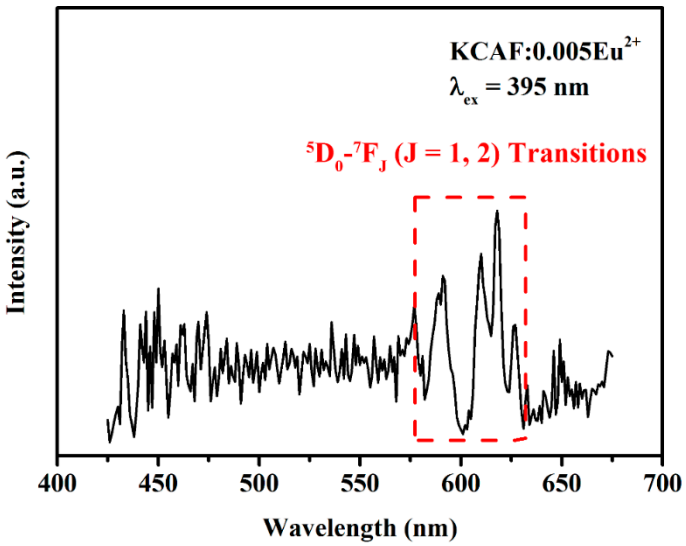



**Figure S5.** PL spectrum of KCAF:0.005$Eu^{2+}$ phosphor ($\lambda_{ex}$ = 395 nm).

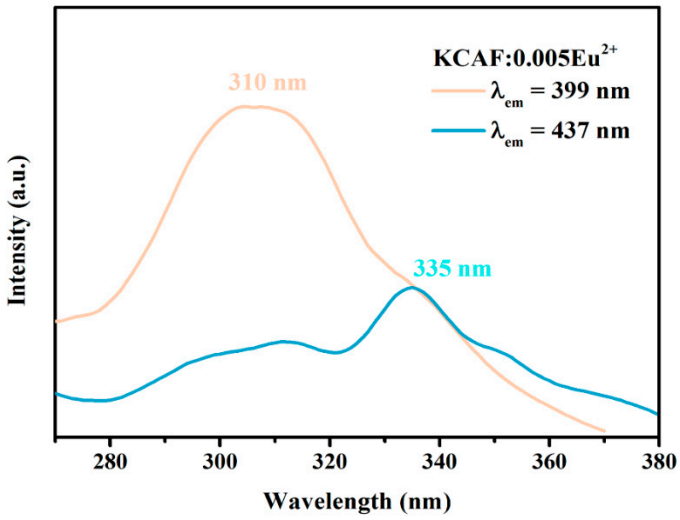



**Figure S6.** PLE spectra of KCAF:0.005$Eu^{2+}$ phosphor monitored at 399 and 437 nm.

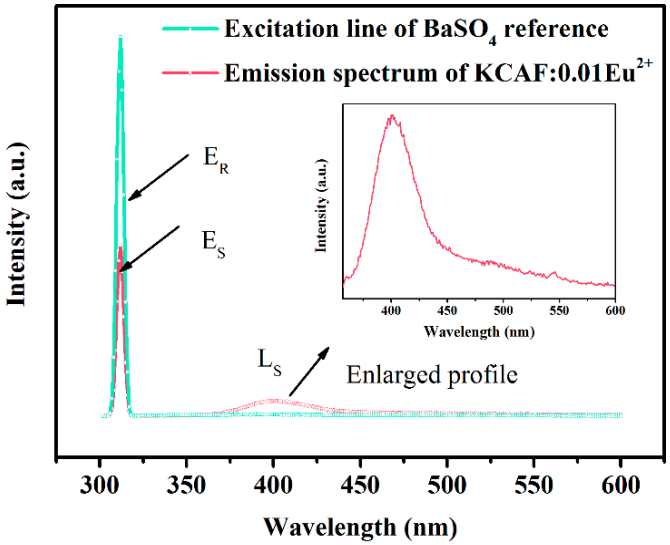



**Figure S7.** Excitation line of $BaSO_4$ and emission spectrum of the KCAF:0.01$Eu^{2+}$ phosphor. The inset is the magnification of the emission spectrum.

[#] Note: In our work, the IQE, absorption efficiency (AE), and EQE values of the phosphor were calculated by the following equations:.

$$IQE = \frac{\int L_S}{\int E_R - \int E_S}$$

$$AE = \frac{\int E_R - \int E_S}{\int E_R}$$

$$EQE = IQE \times AE$$

where $L_S$ is the luminescence emission spectrum of the sample; $E_R$ and $E_S$ are the spectrum of the excitation light without and with the measured sample in the integrating sphere, respectively.

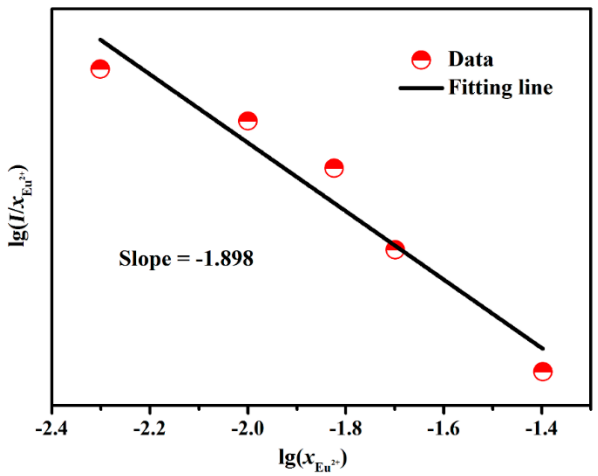



**Figure S8.** Line-fitting relationship of $\lg(I/x_{Eu^{2+}})$ versus $\lg(x_{Eu^{2+}})$.

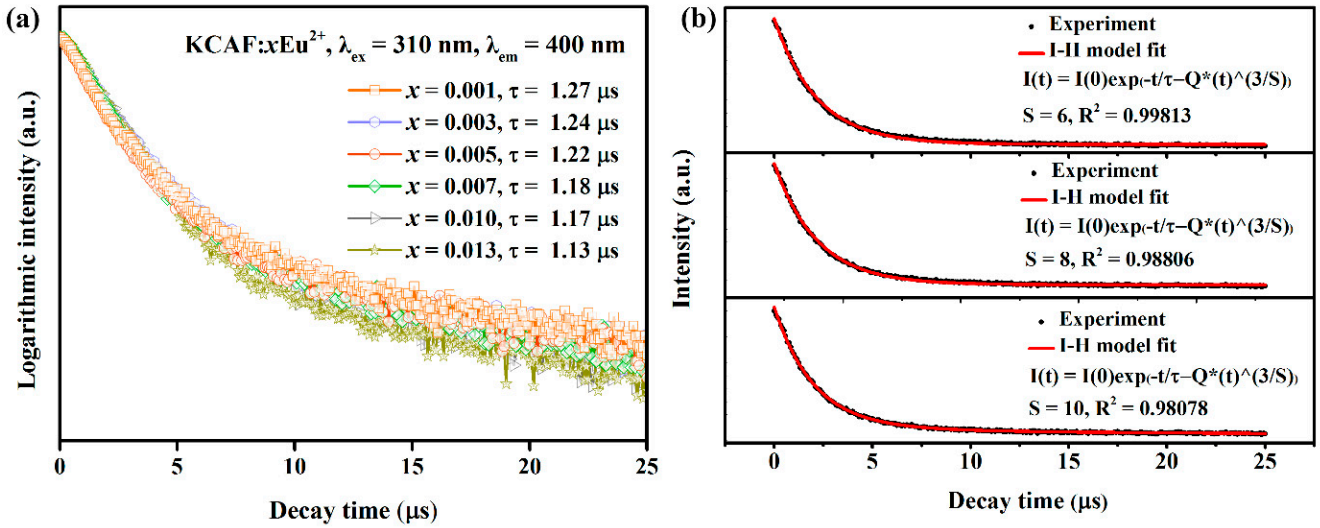



**Figure S9. (a)** The fluorescence decay curves of KCAF:$x$Eu$^{2+}$ ($x$ = 0.001-0.013) phosphors with 310 nm excitation and 400 nm emission. **(b)** The fluorescence decay curves of KCAF:0.005Eu$^{2+}$ phosphor. The solid lines correspond to the fits to the Inokuti-Hirayama model for S = 6, 8, and 10.

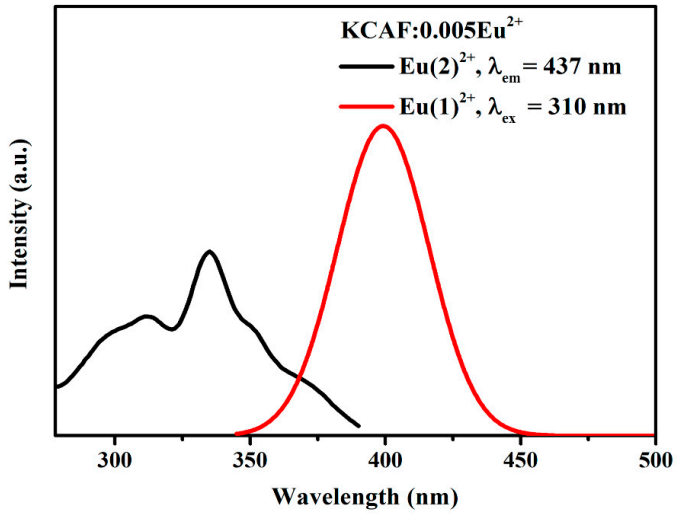



**Figure S10.** The PLE and PL spectra of KCAF:0.005$Eu^{2+}$ phosphor ($\lambda_{em}$ = 437 nm; $\lambda_{ex}$ = 310 nm).

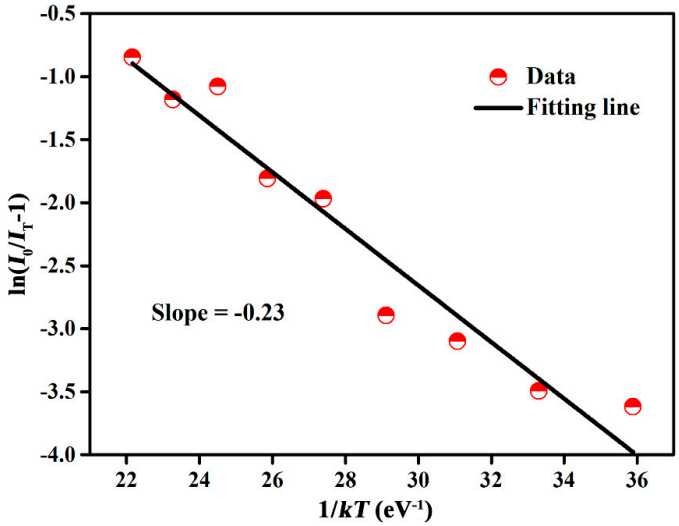



**Figure S11.** The activation energy for thermal quenching of KCAF:0.005$Eu^{2+}$ phosphor.