Multiple sites occupancy induced yellow-orange emission in Eu^{2+}-doped $KSr_6Sc(SiO_4)_4$ phosphor towards optical temperature sensors

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Tables:

Table S1. The atom positions, fraction factors, and occupancy of KSSSO:xEu^{2+} (x=0, x=0.07, x=0.11, 0.13) samples.

Formula			**$KSr_6Sc(SiO_4)_4$**		
Atom	**Wyck**	**x**	**y**	**z**	**Occupancy**
Sr1	8d	0.40961(14)	0.0031(4)	0.3322(5)	0.95
K1	8d	0.40961(14)	0.0031(4)	0.3322(5)	0.05
Sr2	8d	0.22463(15)	0.01748(28)	0.4887(4)	1
Sr3	4c	0.48331(22)	-0.25	-0.0012(8)	1
Sr4	4c	0.3375(4)	0.25	0.7208(8)	0.7
K2	4c	0.3375(4)	0.25	0.7208(8)	0.3
K3	4c	0.31976(33)	-0.25	0.6529(10)	0.6
Sr5	4c	0.31976(33)	-0.25	0.6529(10)	0.4
Sc	4c	0.4937(5)	-0.25	0.4656(14)	1
Si1	4c	0.3300(7)	-0.25	0.2248(20)	1
Si2	4c	0.3586(9)	0.25	0.2385(21)	1
Si3	8d	0.4218(5)	0.0013(13)	0.7839(12)	1
O1	4c	0.3269(15)	-0.25	0.007(4)	1
O2	8d	0.2834(12)	-0.3545(20)	0.352(4)	1
O3	4c	0.3513(25)	-0.25	0.204(8)	1
O4	4c	0.3825(13)	0.25	-0.037(4)	1
O5	8d	0.2945(11)	0.3596(19)	0.2620(23)	1
O6	4c	0.4033(12)	0.25	0.373(4)	1
O7	8d	0.4203(8)	-0.0386(16)	0.9931(28)	1
O8	8d	0.3412(8)	-0.0035(24)	0.7055(21)	1
O9	8d	0.4584(10)	0.1394(16)	0.6785(29)	1
O10	8d	0.4597(11)	-0.0995(18)	0.6930(29)	1

Formula		$KSr_{5.93}Sc(SiO_4)_4:0.07Eu^{2+}$			
Atom	**Wyck**	**x**	**y**	**z**	**Occupancy**
Sr1	8d	0.40798(18)	0.0013(5)	0.3450(5)	0.947
Eu1	8d	0.40798(18)	0.0013(5)	0.3450(5)	0.003
K1	8d	0.40798(18)	0.0013(5)	0.3450(5)	0.05
Sr2	8d	0.22822(18)	0.0201(4)	0.4927(4)	0.986
Eu2	8d	0.22822(18)	0.0201(4)	0.4927(4)	0.014
Sr3	4c	0.48734(30)	-0.25	0.0166(8)	0.978
Eu3	4c	0.48734(30)	-0.25	0.0166(8)	0.022
Sr4	4c	0.3372(4)	0.25	0.7171(8)	0.681
Eu4	4c	0.3372(4)	0.25	0.7171(8)	0.019
K2	4c	0.3372(4)	0.25	0.7171(8)	0.3
K3	4c	0.3198(6)	-0.25	0.7301(16)	0.6
Sr5	4c	0.3198(6)	-0.25	0.7301(16)	0.387
Eu5	4c	0.3198(6)	-0.25	0.7301(16)	0.013
Sc	4c	0.5054(5)	-0.25	0.4944(14)	1
Si1	4c	0.3258(13)	-0.25	0.2310(33)	1
Si2	4c	0.3708(7)	0.25	0.2483(20)	1
Si3	8d	0.4183(6)	-0.0097(14)	0.7766(12)	1
O1	4c	0.3738(16)	-0.25	-0.069(5)	1
O2	8d	0.3071(10)	-0.3364(20)	0.3941(34)	1
O3	4c	0.3686(17)	-0.25	0.248(5)	1
O4	4c	0.3391(22)	0.25	0.091(5)	1
O5	8d	0.2606(9)	0.3466(16)	0.2124(18)	1
O6	4c	0.4027(7)	0.25	0.3910(17)	1
O7	8d	0.4135(6)	-0.0334(11)	1.0194(15)	1
O8	8d	0.3485(7)	0.0311(14)	0.6803(19)	1
O9	8d	0.4745(10)	0.0750(19)	0.7202(25)	1
O10	8d	0.4505(11)	-0.1202(23)	0.6643(33)	1

Formula		$KSr_{5.81}Sc(SiO_4)_4:0.11Eu^{2+}$			
Atom	**Wyck**	**x**	**y**	**z**	**Occupancy**
Sr1	8d	0.40869(24)	-0.0001(5)	0.3317(9)	0.946
Eu1	8d	0.40869(24)	-0.0001(5)	0.3317(9)	0.004
K1	8d	0.40869(24)	-0.0001(5)	0.3317(9)	0.05
Sr2	8d	0.22560(22)	0.0226(4)	0.4930(6)	0.978
Eu2	8d	0.22560(22)	0.0226(4)	0.4930(6)	0.022
Sr3	4c	0.4818(4)	-0.25	-0.0014(12)	0.964
Eu3	4c	0.4818(4)	-0.25	-0.0014(12)	0.036
Sr4	4c	0.3392(5)	0.25	0.7235(10)	0.67
Eu4	4c	0.3392(5)	0.25	0.7235(10)	0.03
K2	4c	0.3392(5)	0.25	0.7235(10)	0.3
K3	4c	0.3213(5)	-0.25	0.6633(14)	0.6
Sr5	4c	0.3213(5)	-0.25	0.6633(14)	0.382
Eu5	4c	0.3213(5)	-0.25	0.6633(14)	0.018
Sc	4c	0.4963(7)	-0.25	0.4761(19)	1
Si1	4c	0.3292(10)	-0.25	0.2295(28)	1
Si2	4c	0.3598(12)	0.25	0.2206(30)	1
Si3	8d	0.4198(8)	0.0029(17)	0.7721(18)	1
O1	4c	0.3288(26)	-0.25	0.046(6)	1
O2	8d	0.2962(12)	-0.3601(22)	0.342(5)	1
O3	4c	0.4055(22)	-0.25	0.316(6)	1
O4	4c	0.3934(20)	0.25	0.062(6)	1
O5	8d	0.2887(13)	0.3475(21)	0.2634(33)	1
O6	4c	0.3992(19)	0.25	0.373(5)	1
O7	8d	0.4185(11)	-0.0338(19)	0.9983(35)	1
O8	8d	0.3350(13)	0.0166(21)	0.680(4)	1
O9	8d	0.4833(13)	0.1063(27)	0.718(4)	1
O10	8d	0.4557(10)	-0.1049(19)	0.6408(33)	1

Formula		**$KSr_{5.81}Sc(SiO_4)_4$:0.13Eu^{2+}**			
Atom	**Wyck**	**x**	**y**	**z**	**Occupancy**
Sr1	8d	0.41164(19)	0.0047(4)	0.3428(5)	0.946
Eu1	8d	0.41164(19)	0.0047(4)	0.3428(5)	0.004
K1	8d	0.41164(19)	0.0047(4)	0.3428(5)	0.05
Sr2	8d	0.22142(18)	0.0114(4)	0.4934(5)	0.973
Eu2	8d	0.22142(18)	0.0114(4)	0.4934(5)	0.027
Sr3	4c	0.48664(31)	-0.25	0.0118(9)	0.958
Eu3	4c	0.48664(31)	-0.25	0.0118(9)	0.042
Sr4	4c	0.3376(5)	0.25	0.7257(8)	0.664
Eu4	4c	0.3376(5)	0.25	0.7257(8)	0.036
K2	4c	0.3376(5)	0.25	0.7257(8)	0.3
K3	4c	0.3168(4)	-0.25	0.6724(11)	0.6
Sr5	4c	0.3168(4)	-0.25	0.6724(11)	0.379
Eu5	4c	0.3168(4)	-0.25	0.6724(11)	0.021
Sc	4c	0.5004(11)	-0.25	0.4862(26)	1
Si1	4c	0.3327(11)	-0.25	0.2461(22)	1
Si2	4c	0.3569(11)	0.25	0.2495(29)	1
Si3	8d	0.4300(4)	0.0012(8)	0.7822(9)	1
O1	4c	0.3487(21)	-0.25	-0.085(5)	1
O2	8d	0.3078(9)	-0.3432(15)	0.3189(23)	1
O3	4c	0.4017(15)	-0.25	0.3860(35)	1
O4	4c	0.3842(21)	0.25	0.178(6)	1
O5	8d	0.2535(7)	0.3387(10)	0.1760(19)	1
O6	4c	0.4073(15)	0.25	0.3903(34)	1
O7	8d	0.4266(6)	-0.0354(9)	1.0177(17)	1
O8	8d	0.3462(7)	0.0281(10)	0.6937(14)	1
O9	8d	0.4488(9)	0.1193(15)	0.7538(22)	1
O10	8d	0.4540(9)	-0.1008(12)	0.6334(22)	1

Table S2. The bond lengths of Sr-O in detail.

Sr1-O2	2.737(23)	Sr3-O9	2.834(21)
Sr1-O3	2.878(25)	Sr3-O9	2.834(21)
Sr1-O5	2.633(22)	Sr3-O10	2.786(21)
Sr1-O6	2.781(5)	Sr3-O10	2.786(21)
Sr1-O7	2.463(19)	**Sr3 Mean**	**2.75**
Sr1-O8	2.759(15)	Sr4-O2	2.856(25)
Sr1-O9	3.043(20)	Sr4-O2	2.856(25)
Sr1-O9	2.690(20)	Sr4-O4	2.324(29)
Sr1-O10	2.938(21)	Sr4-O6	2.701(25)
Sr1-O10	2.732(21)	Sr4-O8	2.840(27)
Sr1-O2	2.737(23)	Sr4-O8	2.840(27)
Sr1 Mean	**2.77**	Sr4-O9	2.843(21)
Sr2-O1	2.786(11)	Sr4-O9	2.843(21)
Sr2-O2	2.953(26)	**Sr4 Mean**	**2.76**
Sr2-O2	2.354(23)	Sr5-O1	2.523(30)
Sr2-O5	2.650(19)	Sr5-O2	2.737(26)
Sr2-O5	2.505(18)	Sr5-O2	2.737(26)
Sr2-O7	2.786(16)	Sr5-O3	3.25(5)
Sr2-O8	2.723(15)	Sr5-O5	2.625(23)
Sr2-O8	2.380(15)	Sr5-O5	2.625(23)
Sr2 Mean	**2.64**	Sr5-O8	2.814(27)
Sr3-O1	2.997(28)	Sr5-O8	2.814(27)
Sr3-O3	2.72(5)	Sr5-O10	3.178(22)
Sr3-O4	2.525(25)	Sr5-O10	3.178(22)
Sr3-O7	2.656(17)	Sr5-O1	2.523(30)
Sr3-O7	2.656(17)	**Sr5 Mean**	**2.85**

Temperature uncertainty δT:

Temperature uncertainty δT determines the temperature measurement accuracy or how small temperature difference sensor can measure. The temperature uncertainty of the nanothermometers δT is defined as:[1-3]

$$\delta T = \frac{1}{S_r} \frac{\delta\Delta}{\Delta} \qquad (S1)$$

where δΔ is the uncertainty in the determination of Δ estimated through the errors in I.

Figures:

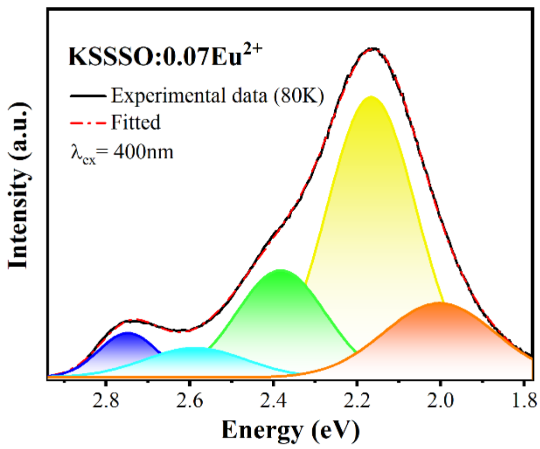

Fig. S1 Gaussian fitting of the PL spectra of KSSSO:$0.07Eu^{2+}$ excited by 400 nm at 80 K.

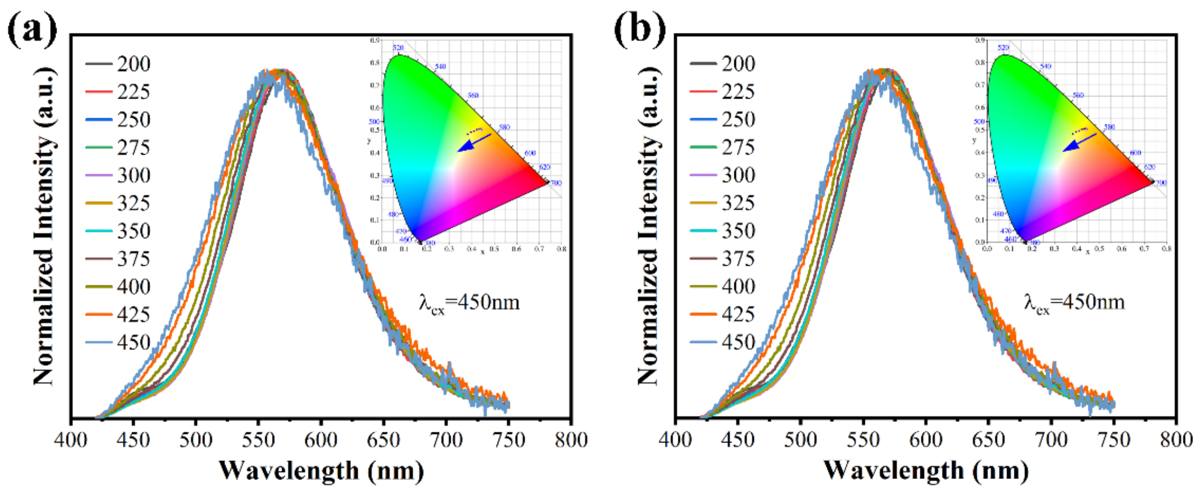

Fig. S2 The normalized TPL spectra excited by 450 (a) and 400 nm (b) and the insets are the CIE chromaticity diagram.

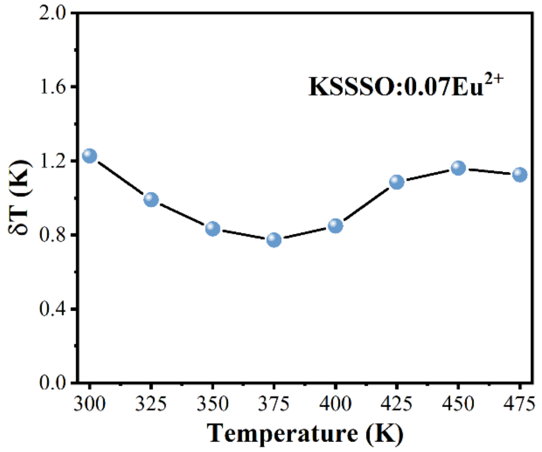

Fig. S3 Temperature uncertainty calculated using Eq. S1.

Reference:

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