Composition-structure-luminescence and enhancement of Cr³⁺

activated broadband near infrared phosphors for night version, bio-

imaging, and noninvasive detection

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Formula	$KSc_{0.97}Cr_{0.03}P_2O_7$
Radiation type	Cu Ka
2θ range (°)	5-130
Step (°)	0.01
$R_{B}(\%)$	2.59
$R_{P}(\%)$	2.88
R_{WP} (%)	4.04
S (%)	1.67
Crystal system	Monoclinic
Space group	$P2_1/c$ (No. 14)
a (Å)	7.4535(1)
b (Å)	10.3481(2)
c (Å)	8.3557(1)
β	106.4860(9)
Volume (Å ³)	617.98(1)
Z	4

Table S1. Crystallographic data, structure refinement parameters of KSPO: 0.03Cr³⁺.

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Atom	Wyck.	Occ.	x/a	y/b	z/c	U [Ų]
K1	4 <i>e</i>	1	0.8193(3)	0.6794(1)	0.9410(2)	0.0000
Sc1	4 <i>e</i>	0.97	0.7643(2)	0.0993(1)	0.7430(2)	0.0000
Cr1	4 <i>e</i>	0.03	0.7643(2)	0.0993(2)	0.7430(2)	0.0000
P1	4 <i>e</i>	1	0.5593(3)	0.3595(3)	0.8108(3)	0.0000
P2	4 <i>e</i>	1	0.8654(3)	0.4011(2)	0.6773(3)	0.0000
01	4 <i>e</i>	1	0.5534(6)	0.2209(5)	0.7662(5)	0.0000
02	4 <i>e</i>	1	0.3650(6)	0.4228(5)	0.7617(6)	0.0000
03	4 <i>e</i>	1	0.6752(6)	0.3912(5)	0.9854(5)	0.0000
O4	4 <i>e</i>	1	0.6595(6)	0.4350(4)	0.6932(5)	0.0000
05	4 <i>e</i>	1	0.9897(6)	0.5053(5)	0.7745(5)	0.0000
06	4 <i>e</i>	1	0.8600(7)	0.4090(5)	0.4981(6)	0.0000
O7	4 <i>e</i>	1	0.9228(6)	0.2652(5)	0.7506(6)	0.0000

Table S2. Atomic parameters of KSPO: 0.03Cr³⁺.

Table S3. Bond length of KSPO: $0.03Cr^{3+}$.

Atom1	Atom2	Symmetry operator	Bond length (Å)
K1	05	x, y, z	2.792(5)
	07	2-x, 1-y, 2-z	2.802(4)
	01	1-x, 0.5+y, 1.5-z	2.858(4)
	07	2-x, 0.5+y, 1.5-z	2.965(5)
	05	2-x, 1-y, 2-z	3.068(4)
	02	1-x, 0.5+y, 1.5-z	3.127(5)
	O3	x, y, z	3.227(5)
	Average leng	gth	2.935
Sc1 Cr1	O6	x, 0.5-y, 0.5+z	2.049(5)
	O2	1-x, -0.5+y, 1.5-z	2.060(5)
	01	x, y, z	2.065(5)
	03	x, 0.5-y, -0.5+z	2.067(4)
	07	x, y, z	2.075(5)
	05	2-x, -0.5+y, 1.5-z	2.117(5)
	Average leng	yth	2.072
P1	01	x, y, z	1.479(6)
	O3	x, y, z	1.506(4)
	02	x, y, z	1.535(5)
	O4	x, y, z	1.597(5)
	Average length		1.529
P2	O6	x, y, z	1.489(5)
	05	x, y, z	1.501(5)
	07	x, y, z	1.545(5)
	O4	x, y, z	1.616(5)
	Average leng	yth	1.538



Fig. S1 The binding energy peaks splitting results of K (a) and Sc (b). The peaks at 293.4, 296.1, and 377.8 eV are attributed to the K $2p_{3/2}$, K $2p_{1/2}$, and K 2s. And the peaks at 404.5, 408.3, and 502.7 eV can be assigned to the Sc $2p_{3/2}$, Sc $2p_{1/2}$, and Sc 2s.



Fig. S2 PLE spectra of KSPO: xCr^{3+} phosphors monitored at 873 nm.



Fig. S3 PL spectra with $BaSO_4$ as the reference under 475 nm excitation for quantum efficiency measurements of KSPO: $0.03Cr^{3+}$.



Fig. S4 XRD pattern of KSPO: $0.03Cr^{3+}$, yYb^{3+} samples. (b) The refinement result of KSPO: $0.03Cr^{3+}$, $0.01Yb^{3+}$. The EDS (c) and SEM mapping (d) of KSPO: $0.03Cr^{3+}$, $0.01Yb^{3+}$.



Fig. S5 The decay curves of Cr^{3+} emission in KSPO: $0.03Cr^{3+}$, yYb^{3+} samples.