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Supplementary Information

Highly Efficient and Thermally Stable Broadband Near-Infrared Emitting Fluoride $Cs_2KGaF_6:Cr^{3+}$ for Multiple LED Applications

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Table S1 The doping concentration of Cr^{3+} measured by ICP optical emission spectroscopy.

Theoretical concentration/mol%	Actual concentration/mol%
1%	1.08%
5%	4.81%
10%	10.89%
15%	16.02%
20%	21.12%

Table S2 Atomic coordinates and isotropic displacement parameters (Å^2) for $Cs_2KGa_{1-x}F_6$:xCr^{3+} (x=0-21.12%).

Cr^{3+} content	atom	*x*	*y*	*z*	B_{iso}	*Occ.*
0%	Cs	0.25	0.25	0.25	1.97	1
	K	0.5	0.5	0.5	1.84	1
	Ga	0	0	0	1.07	1
	F	0.209981	0	0	2.21	1
1.08%	Cs	0.25	0.25	0.25	1.84	1
	K	0.5	0.5	0.5	2.14	1
	Ga	0	0	0	1.10(5)	0.9635
	F	0.213307	0	0	2.70	1
	Cr	0	0	0	0.95(5)	0.0365
4.81%	Cs	0.25	0.25	0.25	2.03	1
	K	0.5	0.5	0.5	1.42	1
	Ga	0	0	0	1.41(5)	0.9580
	F	0.210291	0	0	2.03	1
	Cr	0	0	0	0.92(5)	0.0420
10.89%	Cs	0.25	0.25	0.25	2.17	1
	K	0.5	0.5	0.5	1.58	1
	Ga	0	0	0	1.30(5)	0.9209
	F	0.231395	0	0	1.98	1
	Cr	0	0	0	0.77(5)	0.0791
16.02%	Cs	0.25	0.25	0.25	1.95	1
	K	0.5	0.5	0.5	1.49	1
	Ga	0	0	0	1.37(5)	0.9110
	F	0.213161	0	0	2.24	1
	Cr	0	0	0	0.87(5)	0.0890
21.12%	Cs	0.25	0.25	0.25	1.79	1
	K	0.5	0.5	0.5	1.81	1
	Ga	0	0	0	1.16	0.880(18)
	F	0.214594	0	0	2.77	1
	Cr	0	0	0	0.83	0.120(18)

Table S3 Rietveld refinement data for $Cs_2KGa_{1-x}F_6$:$x$$Cr^{3+}$ (x=0-21.12%).

Cr^{3+} content	**Space group**	***a*** **(Å)**	**α=β=γ (°)**	***Z***	***V*** **(Å^3)**	**R_{wp}/R_p/χ^2**
0%	$Fm\bar{3}m$	8.989610(20)	90	4	726.4781(28)	7.07%/5.39%/3.150
1.08%		8.988504(20)			726.2101(28)	8.17%/5.78%/4.125
4.81%		8.986817(19)			725.8013(27)	7.54%/5.50%/3.467
10.89%		8.985558(25)			725.4961(25)	7.57%/5.50%/3.448
16.02%		8.985383(18)			725.4539(25)	7.62%/5.42%/3.568
21.12%		8.985026(20)			725.3674(28)	7.71%/5.49%/3.552

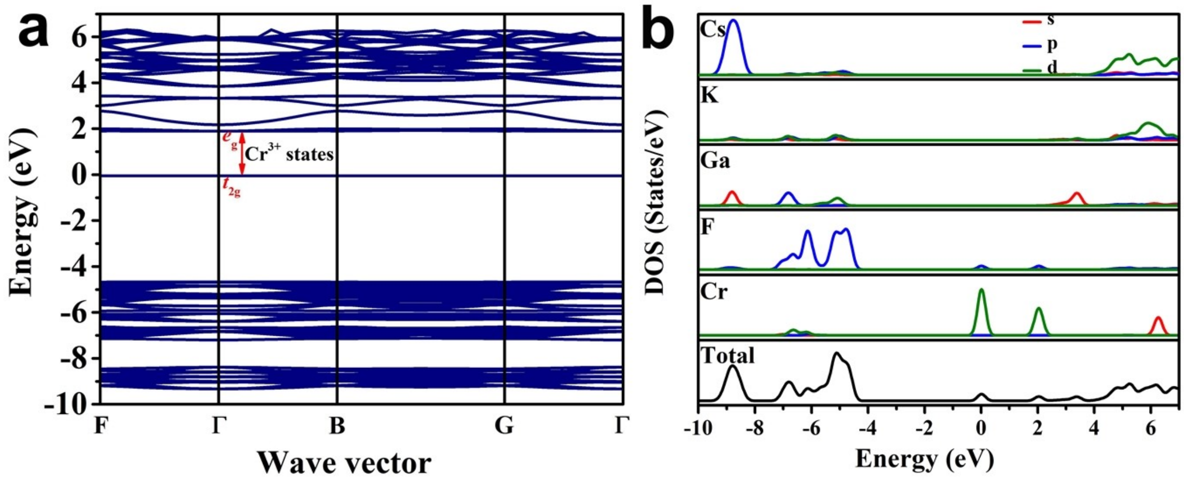

Fig. S1 (a) Band structure and (b) TDOS and PDOS of $Cs_2KGaF_6:Cr^{3+}$.

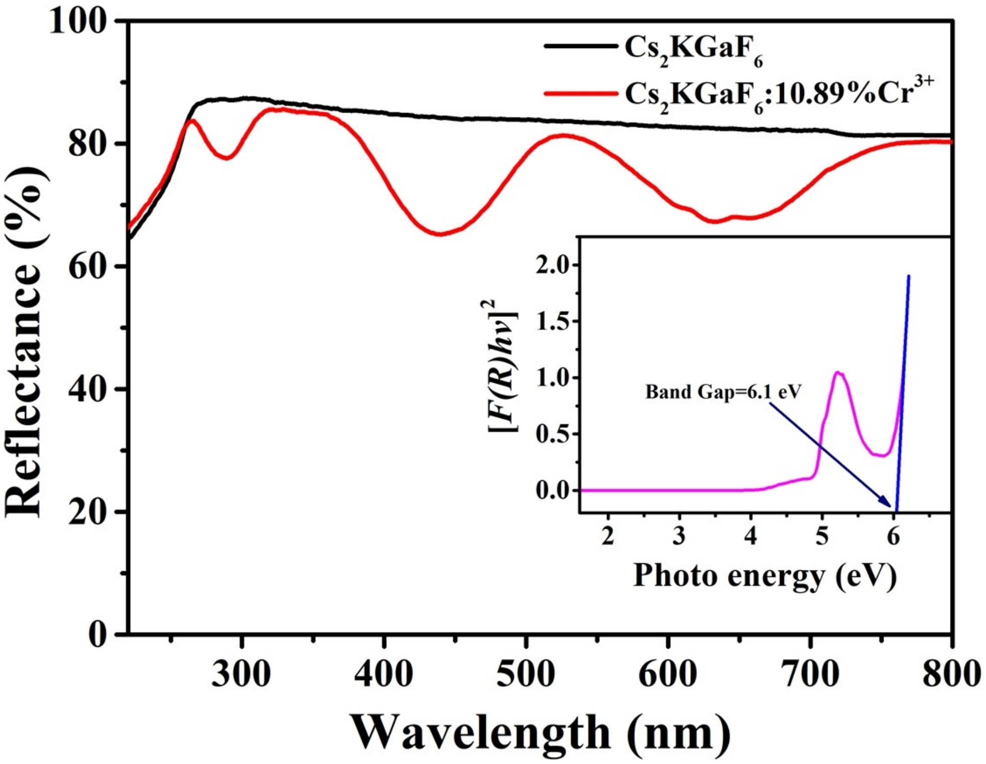

Fig. S2 DRS of Cs_2KGaF_6 and Cs_2KGaF_6:10.89%Cr^{3+}. The inset shows the band gap calculation of Cs_2KGaF_6.

Table S4 The decay curves fitting data of $Cs_2KGa_{1-x}F_6$:$x$$Cr^{3+}$ (x=0-21.12%).

Cr^{3+} content	**A_1**	**τ_1**	**A_2**	**τ_2**	**τ**
1.08%	0.44648	0.26975	0.44648	0.26975	0.26975
4.81%	0.43527	0.26383	0.43527	0.26383	0.26383
10.89%	0.83826	0.26104	0.09991	0.05308	0.25612
16.02%	0.63487	0.28074	0.29694	0.09754	0.25513
21.12%	0.66835	0.26531	0.31266	0.07371	0.24328

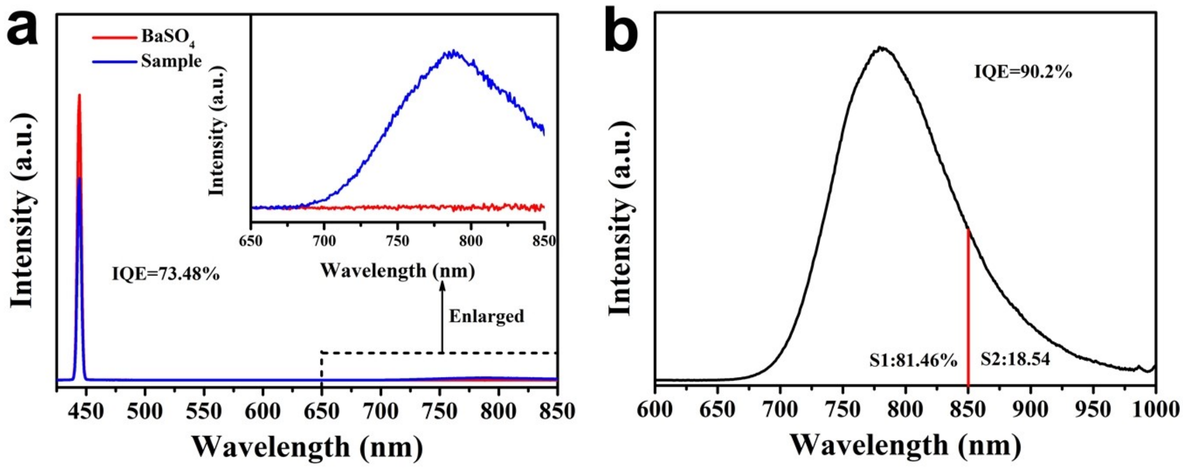

Fig. S3 (a) Excitation and emission spectra of $BaSO_4$ and phosphor sample Cs_2KGaF_6:10.89%Cr^{3+}. (b) Emission spectrum of Cs_2KGaF_6:10.89%Cr^{3+}. The S1 and S2 in Fig. S2b present the emission spectrum parts of 600-850 nm and 850-1000 nm, respectively. The integrated emission intensity ratios of S1 and S2 to that of (S1+S2) are calculated to be about 81.46% and 18.54%, respectively. Meanwhile, the IQE of S1 is determined as 73.48%, thus the IQE of the whole NIR emission of the sample can be calculate as 73.48%/81.54% ≈ 90.2%.

Table S5 PL properties of some Cr^{3+}-activated phosphors and photoelectric properties of the fabricated NIR pc-LEDs.

Phosphor	λ_{ex} (nm)	λ_{em} (nm)	FWHM (nm)	$I_{150°C}$ (%)	IQE (%)	Input power (mW)	NIR output power (mW)@photoelectric efficiency	Ref.
$BaMgAl_{10}O_{17}:Cr^{3+}$	398	762	92.6	63	94	-	3.4@-	1
$InBO_3:Cr^{3+}$	480	820	138	50	46.3	360	37.5@10.42%	2
$LiScP_2O_7:Cr^{3+}$	470	880	170	20	38	300	19@7%	3
$LiScP_2O_7:Cr^{3+},Yb^{3+}$	470	880	210	60	74	300	36@12%	3
$YAl_3(BO_3)_4:Cr^{3+},Yb^{3+}$	450	-	-	80	-	300	26@8.6%	4
$Ca_2LuZr_2Al_3O_{12}:Cr^{3+}$	460	754	117	60	69	60	2.448@4.1%	5
$NaInGe_2O_6:Cr^{3+}$	480	900	175	25	34	-	25@4.85%	6
$Ca_9Ga(PO_4)_7:Cr^{3+}$	440	735	-	68.5	55.7	-	-	7
$CaSc_{1-x}Al_{1+x}SiO_6: Cr^{3+}$	460	950	205	~54	30	-	-	8
$Y_2CaAl_4SiO_{12}:Cr^{3+}$	440	760	160	90.6	90.1	300	62.6@21.2%	8
$Ca_{3-x}Lu_xGa_{2+x}Ge_{3-x}O_{12}:Cr^{3+}$	460	803	267	90	-	300	27.1@16.3%	10
$ScBO_3:Cr^{3+}$	450	800	120	51	65	371	26@7%	11
$Ca_3Sc_2Si_3O_{12}:Cr^{3+}$	460	770	110	97.4	92.3	2892	109.9@3.8%	12
$K_3GaF_6:Cr^{3+}$	442	750	-	-	28	1050	8@<1%	13
$K_3ScF_6:Cr^{3+}$	432	770	120	87.3	71.7	350	32.56564@9.315	14
$K_3AlF_6:Cr^{3+}$	430	763	112	-	31.4	1050	5.5@<1%	15
$K_2NaScF_6:Cr^{3+}$	435	765	100	89.6	74	1094	159.72@14.6%	16
$ScF_3:Cr^{3+}$	468	853	140	85.5	45	110	3.51@3.19%	17
$Na_3ScF_6:Cr^{3+}$	436	774	108	30	91.5	-	699.8@15.46%	18
						52.68	**11.26@21.37%**	
$Cs_2KGaF_6:Cr^{3+}$	**439**	**782**	**110**	**88.7**	**90.2**	**277.5**	**61.18@22.05%**	**This**
						972.8	**183.81@18.89%**	**work**

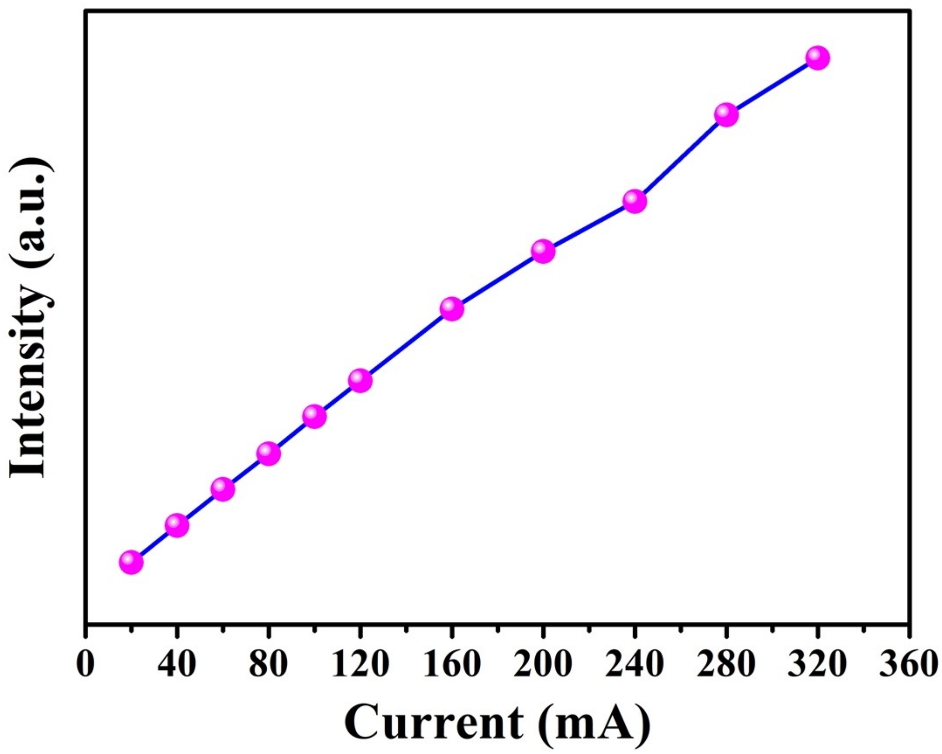

Fig. S4 Driven current dependent integrated NIR intensity.

Table S6 Some photoelectric parameters of the fabricated NIR pc-LED under various driven currents.

Current (mA)	Input electrical power (mW)	NIR output power (mW)	Photoelectric conversion efficiency (%)
20	52.68	11.26	21.37
40	107.20	23.84	22.24
60	160.19	36.28	22.64
80	217.17	48.45	22.31
100	277.50	61.18	22.05
120	336.12	73.44	21.85
160	456.64	98.01	21.46
200	580.00	117.63	20.28
240	707.76	134.71	19.03
280	838.32	164.39	19.61
320	972.80	183.808	18.89

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