Supporting Information

Lanthanide-Doped $NaScF_4$ Nanoprobes: Crystal Structure, Optical Spectroscopy and Biodetection

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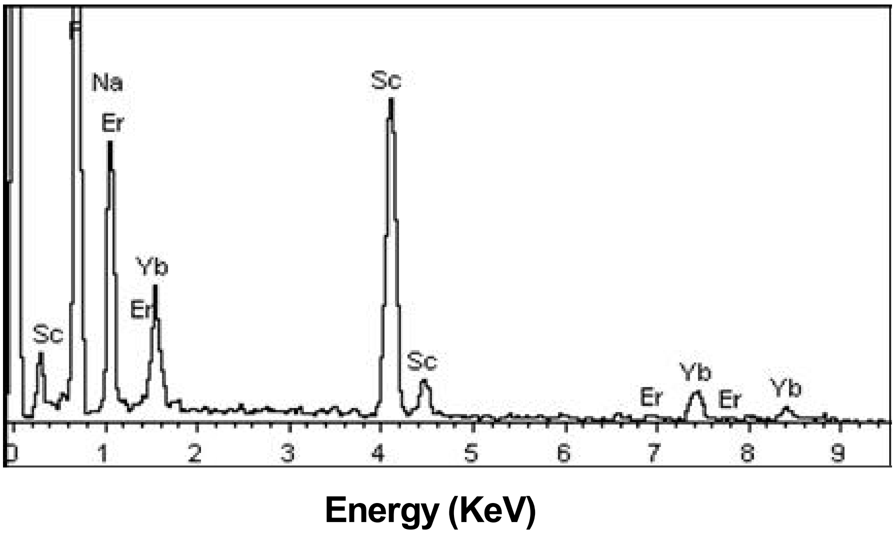

Fig. S1 Energy dispersive X-ray (EDX) spectrum analysis of $NaScF_4$:0.02Er^{3+}/0.18Yb^{3+} NPs, revealing successfully doping of Er^{3+}/Yb^{3+} into $NaScF_4$ host.

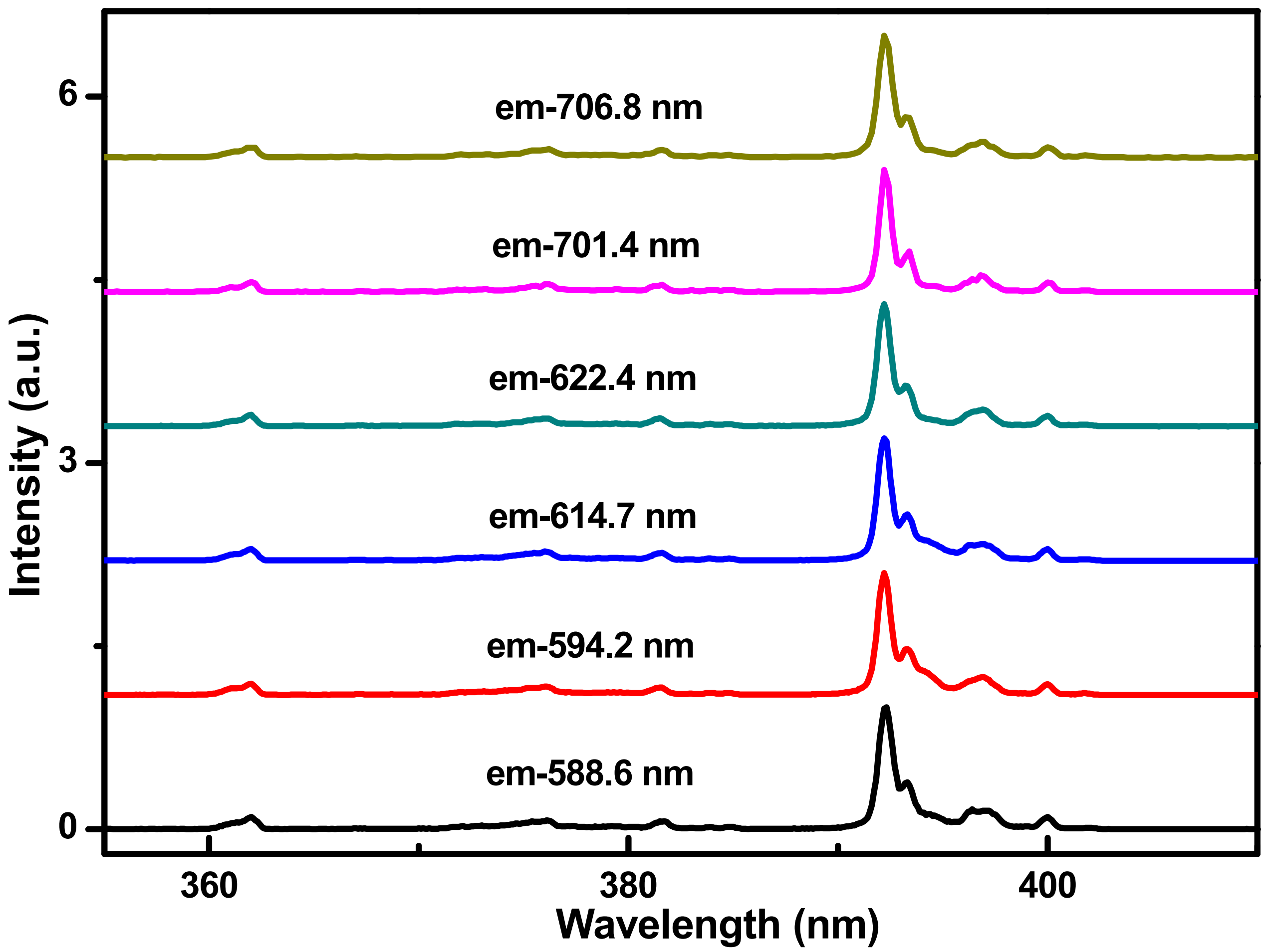

Fig. S2 10 K PL excitation spectra of Eu^{3+} at site B in $NaScF_4$ microcrystals by monitoring the emissions at 588.6, 594.2, 614.7, 622.4, 701.4 and 706.8 nm, respectively.

Table S1. Selected Bond Lengths (Å) and Angles (Å) for $NaScF_4$

Sc(1)-F(3)	2.009(4)	Sc(4)-F(13)	1.997(4)
Sc(1)-F(12)#1	2.053(3)	Sc(4)-F(14)	2.022(4)
Sc(1)-F(4)#2	2.061(3)	Sc(4)-F(11)	2.054(4)
Sc(1)-F(2)#3	2.078(3)	Sc(4)-F(15)	2.077(4)
Sc(1)-F(2)	2.098(3)	Sc(4)-F(17)	2.082(4)
Sc(1)-F(20)#4	2.099(4)	Sc(4)-F(16)	2.114(4)
Sc(1)-F(1)	2.117(3)	Sc(4)-F(10)#6	2.165(4)
Sc(2)-F(5)	2.018(4)	Sc(5)-F(24)#7	2.029(4)
Sc(2)-F(6)	2.019(4)	Sc(5)-F(19)	2.039(4)
Sc(2)-F(4)	2.053(4)	Sc(5)-F(22)#8	2.053(4)
Sc(2)-F(7)	2.087(4)	Sc(5)-F(18)	2.073(4)
Sc(2)-F(3)	2.111(3)	Sc(5)-F(17)	2.106(4)
Sc(2)-F(8)	2.123(4)	Sc(5)-F(16)	2.113(4)
Sc(2)-F(12)#5	2.139(4)	Sc(5)-F(18)#8	2.105(4)
Sc(3)-F(10)	2.034(4)	Sc(6)-F(21)	2.019(4)
Sc(3)-F(9)	2.041(4)	Sc(6)-F(23)	2.024(4)
Sc(3)-F(15)#6	2.039(4)	Sc(6)-F(22)	2.065(4)
Sc(3)-F(11)	2.053(4)	Sc(6)-F(1)#9	2.089(4)
Sc(3)-F(7)	2.099(4)	Sc(6)-F(24)	2.096(4)
Sc(3)-F(8)	2.114(4)	Sc(6)-F(20)	2.118(4)
Sc(3)-F(9)#6	2.142(5)	Sc(6)-F(19)	2.137(4)
F(3)-Sc(1)-F(12)#1	173.73(15)	F(13)-Sc(4)-F(14)	171.90(18)
F(3)-Sc(1)-F(4)#2	102.73(17)	F(13)-Sc(4)-F(11)	80.06(18)
F(12)#1-Sc(1)-F(4)#2	82.54(15)	F(14)-Sc(4)-F(11)	93.89(18)
F(3)-Sc(1)-F(2)#3	86.16(15)	F(13)-Sc(4)-F(15)	84.45(17)
F(12)#1-Sc(1)-F(2)#3	92.20(13)	F(14)-Sc(4)-F(15)	89.29(19)
F(4)#2-Sc(1)-F(2)#3	73.25(14)	F(11)-Sc(4)-F(15)	80.88(17)
F(3)-Sc(1)-F(2)	78.27(13)	F(13)-Sc(4)-F(17)	81.29(17)
F(12)#1-Sc(1)-F(2)	106.57(15)	F(14)-Sc(4)-F(17)	106.81(17)
F(4)#2-Sc(1)-F(2)	75.57(14)	F(11)-Sc(4)-F(17)	134.40(18)
F(2)#3-Sc(1)-F(2)	140.91(14)	F(15)-Sc(4)-F(17)	137.76(18)
F(3)-Sc(1)-F(20)#4	89.39(16)	F(13)-Sc(4)-F(16)	99.52(17)
F(12)#1-Sc(1)-F(20)#4	88.01(16)	F(14)-Sc(4)-F(16)	83.70(17)
F(4)#2-Sc(1)-F(20)#4	145.66(17)	F(11)-Sc(4)-F(16)	155.33(19)
F(2)#3-Sc(1)-F(20)#4	140.34(15)	F(15)-Sc(4)-F(16)	74.56(15)
F(2)-Sc(1)-F(20)#4	75.68(14)	F(17)-Sc(4)-F(16)	68.99(13)
F(3)-Sc(1)-F(1)	92.00(16)	F(13)-Sc(4)-F(10)#7	103.45(18)
F(12)#1-Sc(1)-F(1)	81.74(14)	F(14)-Sc(4)-F(10)#7	79.67(16)
F(4)#2-Sc(1)-F(1)	141.17(16)	F(11)-Sc(4)-F(10)#7	73.05(17)
F(2)#3-Sc(1)-F(1)	72.14(13)	F(15)-Sc(4)-F(10)#7	150.77(17)
F(2)-Sc(1)-F(1)	143.12(15)	F(17)-Sc(4)-F(10)#7	71.47(16)
F(20)#4-Sc(1)-F(1)	68.66(14)	F(16)-Sc(4)-F(10)#7	130.02(18)

F(5)-Sc(2)-F(6)	169.71(17)	F(24)#7-Sc(5)-F(19)	173.47(16)
F(5)-Sc(2)-F(4)	92.98(15)	F(24)#7-Sc(5)-F(22)#8	100.91(18)
F(6)-Sc(2)-F(4)	81.09(15)	F(19)-Sc(5)-F(22)#8	84.87(17)
F(5)-Sc(2)-F(7)	82.58(17)	F(24)#7-Sc(5)-F(18)	77.72(15)
F(6)-Sc(2)-F(7)	98.42(17)	F(19)-Sc(5)-F(18)	106.79(18)
F(4)-Sc(2)-F(7)	150.58(17)	F(22)#8-Sc(5)-F(18)	76.64(16)
F(5)-Sc(2)-F(3)	86.49(15)	F(24)#7-Sc(5)-F(17)	90.98(18)
F(6)-Sc(2)-F(3)	84.02(16)	F(19)-Sc(5)-F(17)	82.63(16)
F(4)-Sc(2)-F(3)	77.58(15)	F(22)#8-Sc(5)-F(17)	138.76(18)
F(7)-Sc(2)-F(3)	73.13(15)	F(18)-Sc(5)-F(17)	144.59(16)
F(5)-Sc(2)-F(8)	107.56(16)	F(24)#7-Sc(5)-F(16)	87.68(16)
F(6)-Sc(2)-F(8)	82.19(16)	F(19)-Sc(5)-F(16)	88.73(18)
F(4)-Sc(2)-F(8)	139.49(17)	F(22)#8-Sc(5)-F(16)	150.18(19)
F(7)-Sc(2)-F(8)	68.52(14)	F(18)-Sc(5)-F(16)	77.44(16)
F(3)-Sc(2)-F(8)	136.57(15)	F(17)-Sc(5)-F(16)	68.56(14)
F(5)-Sc(2)-F(12)#5	80.75(15)	F(24)#7-Sc(5)-F(18)#8	86.68(17)
F(6)-Sc(2)-F(12)#5	105.81(16)	F(19)-Sc(5)-F(18)#8	92.30(16)
F(4)-Sc(2)-F(12)#5	76.63(14)	F(22)#8-Sc(5)-F(18)#8	71.92(16)
F(7)-Sc(2)-F(12)#5	130.56(17)	F(18)-Sc(5)-F(18)#8	141.38(16)
F(3)-Sc(2)-F(12)#5	150.48(14)	F(17)-Sc(5)-F(18)#8	69.51(15)
F(8)-Sc(2)-F(12)#5	72.91(14)	F(16)-Sc(5)-F(18)#8	137.55(16)
F(10)-Sc(3)-F(9)	107.0(2)	F(21)-Sc(6)-F(23)	172.32(16)
F(10)-Sc(3)-F(15)#6	173.30(19)	F(21)-Sc(6)-F(22)	79.01(18)
F(9)-Sc(3)-F(15)#6	78.03(17)	F(23)-Sc(6)-F(22)	94.51(18)
F(10)-Sc(3)-F(11)	83.17(18)	F(21)-Sc(6)-F(1)#9	100.54(16)
F(9)-Sc(3)-F(11)	76.66(17)	F(23)-Sc(6)-F(1)#9	83.04(15)
F(15)#6-Sc(3)-F(11)	102.47(18)	F(22)-Sc(6)-F(1)#9	150.40(18)
F(10)-Sc(3)-F(7)	82.64(18)	F(21)-Sc(6)-F(24)	83.27(15)
F(9)-Sc(3)-F(7)	144.45(18)	F(23)-Sc(6)-F(24)	91.49(18)
F(15)#6-Sc(3)-F(7)	90.70(19)	F(22)-Sc(6)-F(24)	78.80(16)
F(11)-Sc(3)-F(7)	138.9(2)	F(1)#9-Sc(6)-F(24)	71.81(15)
F(10)-Sc(3)-F(8)	89.02(19)	F(21)-Sc(6)-F(20)	81.80(15)
F(9)-Sc(3)-F(8)	77.41(17)	F(23)-Sc(6)-F(20)	105.86(16)
F(15)#6-Sc(3)-F(8)	87.84(17)	F(22)-Sc(6)-F(20)	139.03(18)
F(11)-Sc(3)-F(8)	149.3(2)	F(1)#9-Sc(6)-F(20)	68.81(13)
F(7)-Sc(3)-F(8)	68.48(13)	F(24)-Sc(6)-F(20)	134.17(16)
F(10)-Sc(3)-F(9)#6	91.78(17)	F(21)-Sc(6)-F(19)	100.57(17)
F(9)-Sc(3)-F(9)#6	140.98(17)	F(23)-Sc(6)-F(19)	81.39(15)
F(15)#6-Sc(3)-F(9)#6	86.62(19)	F(22)-Sc(6)-F(19)	74.22(16)
F(11)-Sc(3)-F(9)#6	71.95(17)	F(1)#9-Sc(6)-F(19)	133.82(17)
F(7)-Sc(3)-F(9)#6	70.16(15)	F(24)-Sc(6)-F(19)	151.37(15)
F(8)-Sc(3)-F(9)#6	138.15(16)	F(20)-Sc(6)-F(19)	74.23(15)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y+1,z+1/3

#2 -y,x-y+1,z+1/3
#3 -x+y-1,-x,z-1/3
#4 -x+y-1,-x+1,z+2/3
#5 -x+y-1,-x+1,z-1/3
#6 -y+1,x-y+2,z+1/3
#7 -x+y-1,-x+2,z+2/3
#8 -y+2,x-y+3,z+1/3
#9 -y+1,x-y+2,z-2/3

Table S2. Atomic coordinates（$\times 10^4$) and equivalent isotropic displacement parameters U (eq) (Å$^2\times 10^3$) for $NaScF_4$.

Atom	x	y	z	U(eq)
Sc(1)	-2168(1)	3842(1)	7278(1)	4(1)
Sc(2)	-2173(1)	5749(1)	3988(1)	7(1)
Sc(3)	-549(1)	8841(1)	4184(2)	14(1)
Sc(4)	1284(1)	12417(1)	4139(2)	10(1)
Sc(5)	2826(1)	15506(1)	4268(2)	8(1)
Sc(6)	4557(1)	15471(1)	907(1)	7(1)
Na(1)	-3829(3)	5626(3)	7294(3)	23(1)
Na(2)	2710(3)	10508(3)	3896(3)	19(1)
Na(3)	2888(3)	13946(3)	7647(3)	19(1)
Na(4)	4567(3)	13963(3)	4296(3)	19(1)
Na(5)	1221(3)	13870(3)	658(3)	22(1)
Na(6)	2815(3)	12188(3)	888(4)	27(1)
F(1)	-533(3)	4105(3)	6448(4)	13(1)
F(2)	-2910(3)	4566(3)	8681(4)	14(1)
F(3)	-2065(3)	5188(3)	6093(4)	15(1)
F(4)	-3409(3)	3966(3)	3930(4)	22(1)
F(5)	-817(3)	5471(3)	3484(4)	13(1)
F(6)	-3586(3)	5820(3)	4784(4)	15(1)
F(7)	-826(4)	7228(3)	5055(4)	21(1)
F(8)	-1827(4)	7365(3)	2987(4)	20(1)
F(9)	-1235(3)	9595(3)	2840(4)	26(1)
F(10)	760(4)	8756(4)	3075(5)	28(1)
F(11)	686(4)	10624(3)	4282(5)	32(1)
F(12)	4610(3)	12094(3)	5067(4)	11(1)
F(13)	2716(3)	12385(4)	3407(4)	20(1)
F(14)	-302(4)	12240(4)	4710(4)	21(1)
F(15)	651(4)	11919(4)	2049(5)	25(1)
F(16)	1548(4)	13992(3)	3126(4)	17(1)
F(17)	2592(4)	13921(3)	5196(4)	18(1)
F(18)	2090(3)	16219(3)	2883(4)	24(1)
F(19)	4130(3)	15416(3)	3143(4)	17(1)
F(20)	4920(3)	14198(3)	1851(4)	15(1)
F(21)	3102(3)	13985(3)	193(4)	15(1)
F(22)	3288(4)	15986(4)	1017(5)	34(1)
F(23)	5920(3)	17082(3)	1498(4)	18(1)
F(24)	4597(3)	16062(4)	-1207(4)	20(1)

Table S3. Absolute quantum yields (QYs) of the $NaScF_4$:0.02Er^{3+}/0.18Yb^{3+} and $NaYF_4$:0.02Er^{3+}/0.20Yb^{3+} samples.

$NaScF_4$ (this work)		$NaYF_4$ (Ref.1)[1]	
Average particle size/nm	QY (%)	Average particle size/nm	QY (%)
115 ± 11	0.61	100	0.3
41.6 ± 3.5	0.09	30	0.1
19.6 ± 1.3	0.02	10	0.005

1.J.-C. Boyer and F. C. J. M. van Veggel, *Nanoscale*, 2010, **2**, 1417-1419.