

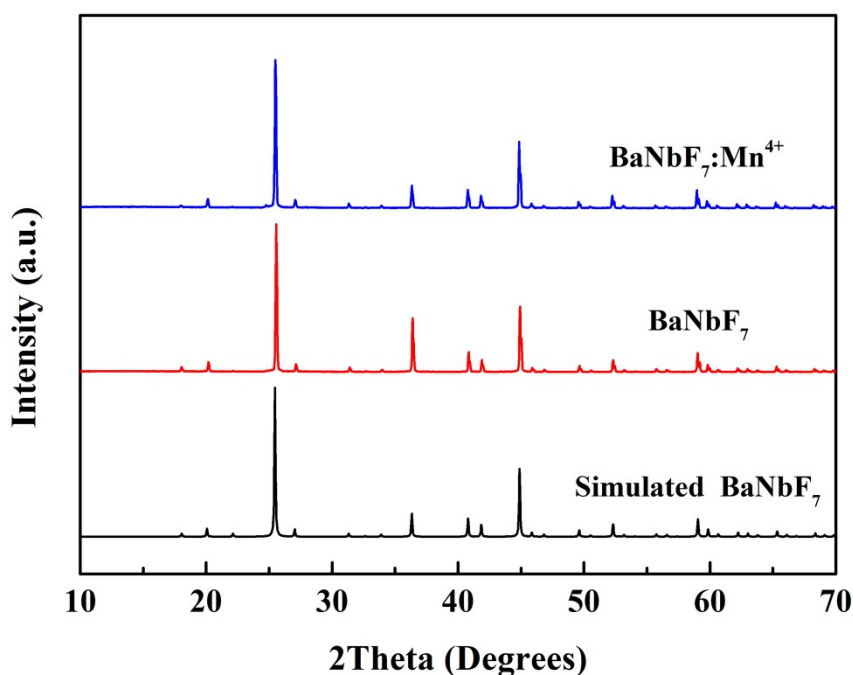
## A Strong Zero-Phonon Line red phosphor $\text{BaNbF}_7:\text{Mn}^{4+}$ for White LEDs

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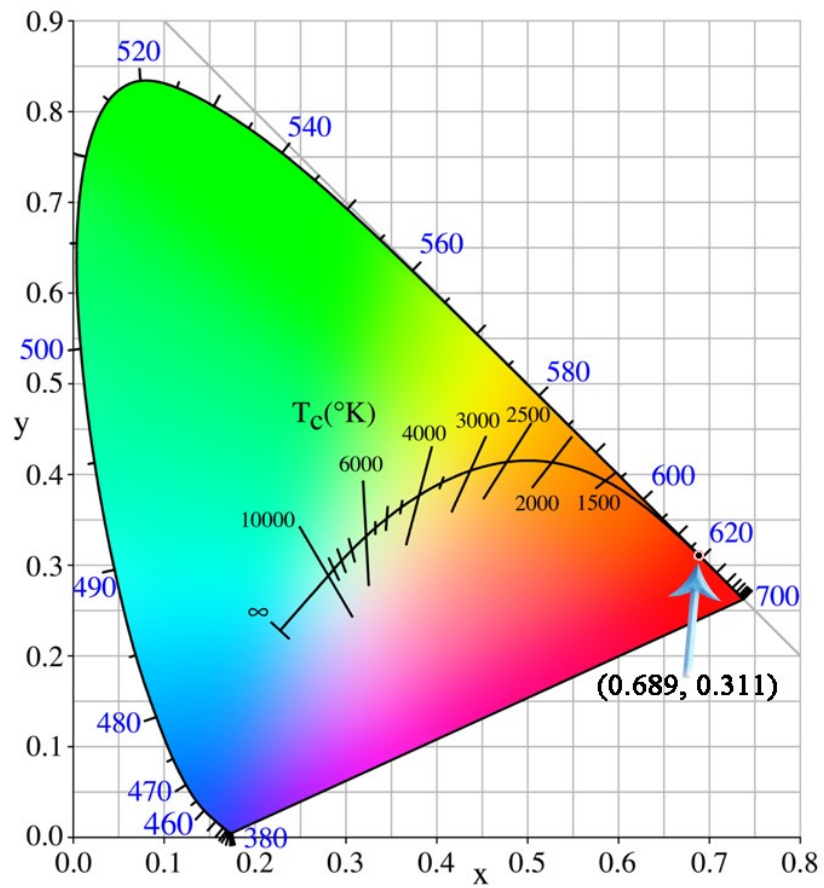
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**Figure. S1.** XRD patterns of  $\text{BaNbF}_7$  and  $\text{BaNbF}_7:\text{Mn}^{4+}$  (0.8mol%  $\text{Mn}^{4+}$ )



**Figure. S2.** CIE chromaticity diagram of BaNbF7: Mn<sup>4+</sup>.

**Table S1.** Atomic displacement parameters ( $\text{\AA}^2$ ) of the  $\text{BaNbF}_7$ 

Atom	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0094 (4)	0.0094 (4)	0.0094 (4)	0.0004 (2)	-0.0004 (2)	-0.0004 (2)
Ba2	0.0112 (4)	0.0112 (4)	0.0112 (4)	0.0012 (2)	-0.0012 (2)	-0.0012 (2)
Nb	0.0106 (3)	0.0106 (3)	0.0106 (3)	0.0001 (3)	0.0001 (3)	-0.0001 (3)
F1	0.0150 (13)	0.0150 (13)	0.0150 (13)	0.0001 (17)	0.0001 (17)	-0.0001 (17)
F2	0.0127 (19)	0.0138 (18)	0.0175 (19)	0.0006 (16)	-0.0028 (17)	-0.0066 (18)
F3	0.0164 (19)	0.017 (2)	0.0136 (18)	0.0016 (17)	-0.0008 (17)	-0.0032 (17)

**Table S2.** Selected bond length and bond angles of  $\text{BaNbF}_7$  based on the crystallographic data

Bond	Length/ $\text{\AA}$	Bond	Length/ $\text{\AA}$
Ba1-F2	2.782(4)	Ba1-F3	2.842(4)
Ba2-F1	2.818(4)	Ba2-F3	2.714(4)
Nb-F1	1.922(4)	Nb-F2	1.914(4)
Nb-F3	2.011(4)		
Bond	Bond angle/ $^\circ$	Bond	Bond angle/ $^\circ$
F2-Ba1-F2	60.06(10)	F2-Ba1-F3	63.17(10)
F2-Ba1-F3	64.41(10)	F3-Ba1-F3	52.85(10)
F1-Ba2-F3	67.89(10)	F3-Ba2-F3	73.30(10)
F1-Nb-F2	78.1(2)	F1-Nb-F3	1334.4(2)
F2-Nb-F2	115.9(2)	F2-Nb-F3	78.56(15)
F2-Nb-F3	76.79(15)	F3-Nb-F3	77.94(14)

**Figure. E1.** Varshni equation as follows:

$$E(T) = E_0 - \frac{aT^2}{T + b} \quad (1)$$

Where  $E(T)$  is the energy difference between the excited state and the ground state at temperature T.