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Effect of Y^{3+} on the local structure and luminescent properties of $La_{3-x}Y_xSi_6N_{11}:Ce^{3+}$ phosphors for high power LED lighting

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Table S1. Atomic coordinates and isotropic displacement parameters of $\text{La}_{2.86-x}\text{Y}_x\text{Si}_6\text{N}_{11} \cdot 0.14\text{Ce}^{3+}$ ($x = 0.1, 0.5, 0.9$) from the Rietveld Refinement of SPD.

$\text{La}_{2.86-x}\text{Y}_x\text{Si}_6\text{N}_{11} \cdot 0.14\text{Ce}^{3+}$ ($x = 0.1$)					
	x	y	z	<i>Occu.</i>	<i>Biso.</i>
La ₍₁₎	0.3187	0.1813	0.6392	0.958	0.675
Y ₍₁₎	0.3187	0.1813	0.6392	0.042	0.675
La ₍₂₎	0	0	0.6554	0.984	0.675
Y ₍₂₎	0	0	0.6554	0.016	0.675
Si ₍₁₎	0.0781	0.2102	0.1229	1.000	0.418
Si ₍₂₎	0.6176	0.1176	0.6103	1.000	0.418
N ₍₁₎	0.0740	0.2288	0.4723	1.000	0.427
N ₍₂₎	0.6542	0.1543	0.9622	1.000	0.427
N ₍₃₎	0	0.1777	0.0204	1.000	0.427
N ₍₄₎	0.5000	0	0.5771	1.000	0.427
$\text{La}_{2.86-x}\text{Y}_x\text{Si}_6\text{N}_{11} \cdot 0.14\text{Ce}^{3+}$ ($x = 0.5$)					
	x	y	z	<i>Occu.</i>	<i>Biso.</i>
La ₍₁₎	0.3187	0.1813	0.6418	0.886	0.662
Y ₍₁₎	0.3187	0.1813	0.6418	0.114	0.662
La ₍₂₎	0	0	0.6651	0.728	0.662
Y ₍₂₎	0	0	0.66651	0.272	0.662
Si ₍₁₎	0.0765	0.2102	0.1250	1.000	0.400
Si ₍₂₎	0.6183	0.1183	0.6090	1.000	0.400
N ₍₁₎	0.0740	0.2288	0.4723	1.000	0.400
N ₍₂₎	0.6518	0.1518	0.9600	1.000	0.400
N ₍₃₎	0	0.1764	0.0155	1.000	0.400
N ₍₄₎	0.5000	0	0.5673	1.000	0.400

La _{2.86-x} Y _x Si ₆ N ₁₁ :0.14Ce ³⁺ (x = 0.9)					
	x	y	z	Occu.	Biso.
La ₍₁₎	0.3205	0.1795	0.6701	0.743	0.816
Y ₍₁₎	0.3161	0.1838	0.6819	0.257	0.816
La ₍₂₎	0	0	0.6911	0.613	0.816
Y ₍₂₎	0	0	0.6911	0.387	0.816
Si ₍₁₎	0.0770	0.2094	0.1513	1.000	0.400
Si ₍₂₎	0.6179	0.1179	0.6387	1.000	0.400
N ₍₁₎	0.0770	0.2319	0.5085	1.000	0.400
N ₍₂₎	0.6554	0.1554	0.9926	1.000	0.400
N ₍₃₎	0	0.1759	0.0466	1.000	0.400
N ₍₄₎	0.5000	0	0.6077	1.000	0.400

Table S2. Crystallographic Data after Refinements of La_{2.86-x}Y_xSi₆N₁₁:0.14Ce³⁺ (x = 0, 0.1, 0.3, 0.5, 0.7, 0.9)

x	a (Å)	c (Å)	V_{La(1)/Y(1)} (Å³)	V_{La(2)/Y(2)} (Å³)	Bond La₍₂₎-N (Å)
0	10.1885	4.840	28.2793	29.8939	2.6362
0.1	10.1793	4.841	28.1770	29.6197	2.6280
0.3	10.1573	4.840	27.8490	29.2873	2.6146
0.5	10.137	4.847	27.5418	28.9138	2.5987
0.7	10.1231	4.841	27.2333	28.1523	2.5926
0.9	10.1143	4.842	27.1696	27.6786	2.5892

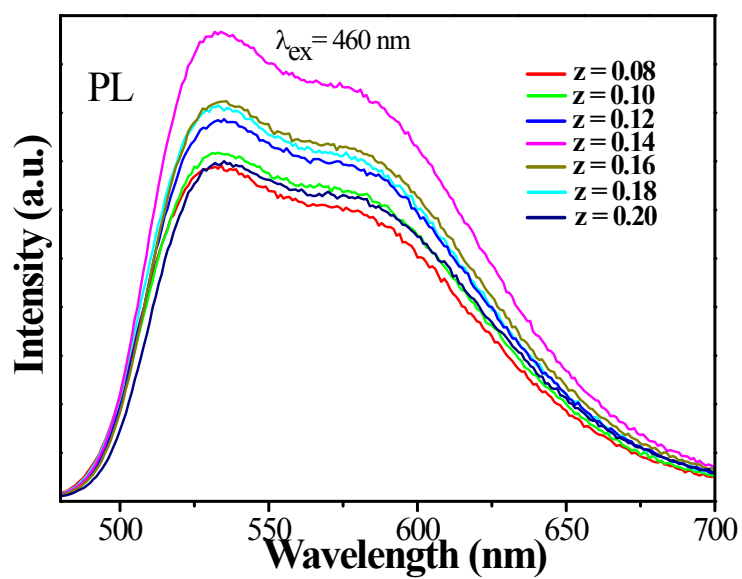


Figure S1. PL spectra of $\text{La}_{3-z}\text{Si}_6\text{N}_{11}:z\text{Ce}^{3+}$ with varying Ce^{3+} concentrations ($z = 0.08, 0.10, 0.12, 0.14, 0.16, 0.18, 0.20$)

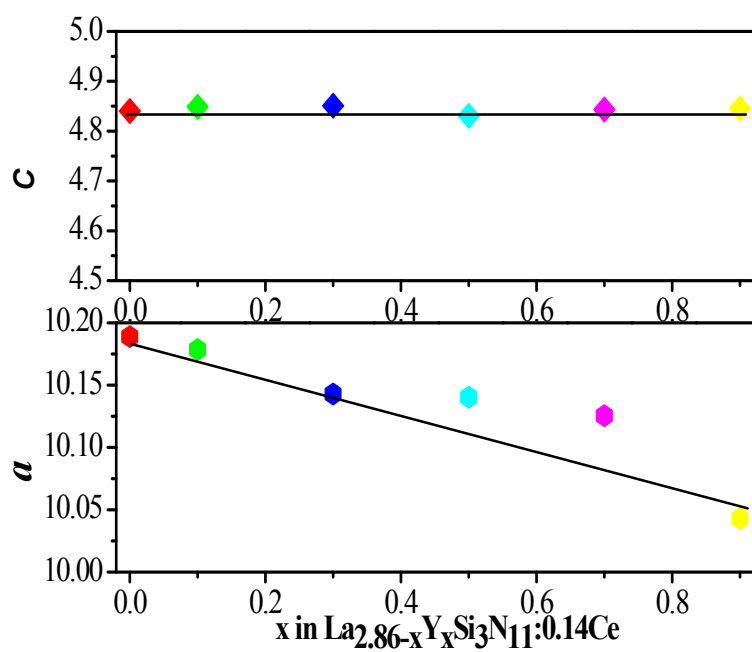


Figure S2. The cell parameters a and c of $\text{La}_{2.86-x}\text{Y}_x\text{Si}_6\text{N}_{11}:0.14\text{Ce}^{3+}$.

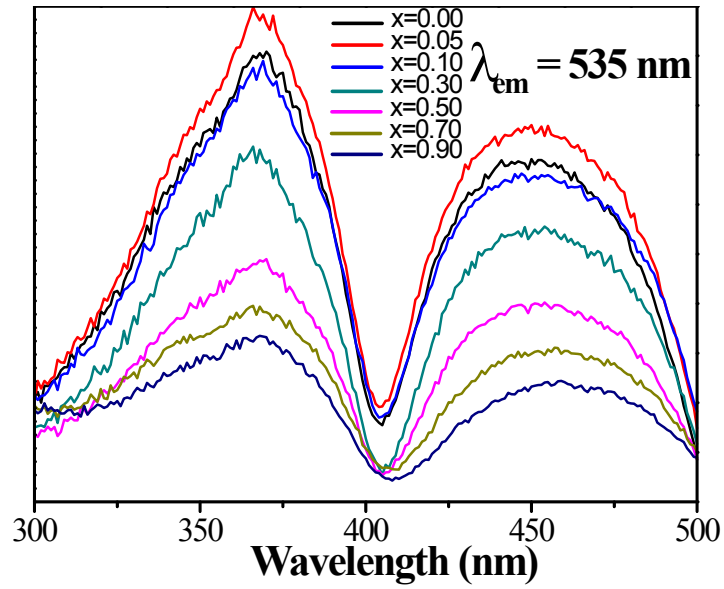


Figure S3. Excitation spectra of $\text{La}_{2.86-x}\text{Y}_x\text{Si}_6\text{N}_{11}:0.14\text{Ce}^{3+}$ ($x = 0, 0.05, 0.1, 0.3, 0.5, 0.7, 0.9$).

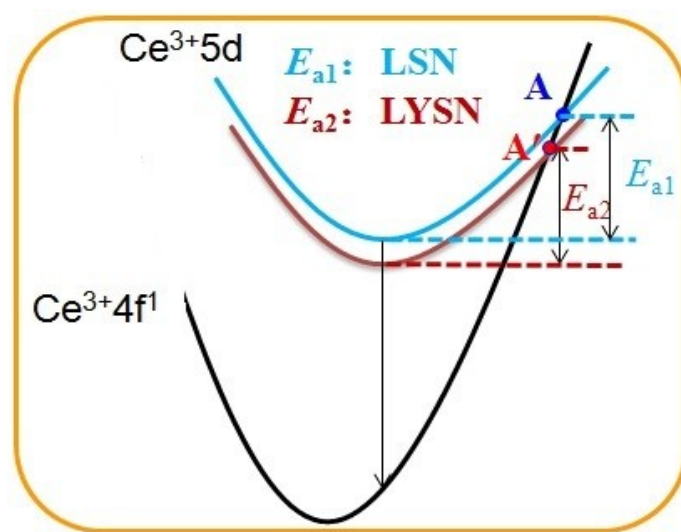


Figure S4. The configurational coordinate of the ground state of Ce^{3+} and the excited states of Ce^{3+} in LSN and LYSN phosphors.