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Crystal structure analysis and evidence of mixed anion coordination at Ce^{3+} site in $Y_3Al_2(Al, Si)_3(O,N)_{12}$ oxynitride garnet phosphor

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Supporting Information

Crystal structure analysis of YASiONG: Ce^{3+} and YAG: Ce^{3+} phosphors by TOF -NPD

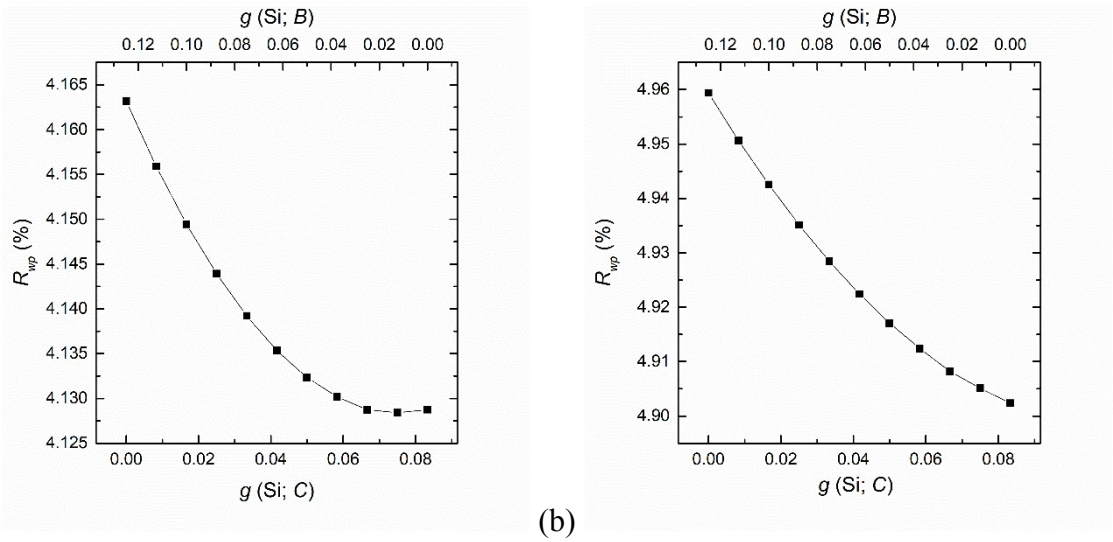

Fig.S1 Variation in R_{wp} value with the occupancy factors of Si at the *B* and *C* sites, *g*(Si;*B*) and *g*(Si;*C*) of YASiONG:Ce measured at (a) 90° and (b) BS banks.

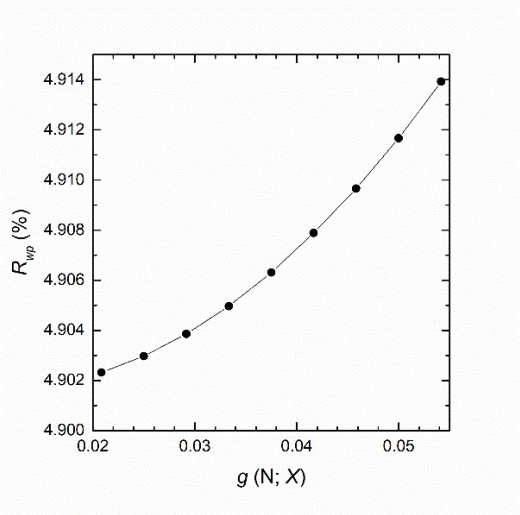

Fig.S2 Variation of R_{wp} value with occupancy factor of N at X site, g(N;X) of YASiONG:Ce measured at BS bank.

Table S1 Results of the structure refinements of YASiONG:Ce ($Y_{2.985}Ce_{0.015}Al_{4.75}Si_{0.25}O_{11.75}N_{0.25}$) based on the nine different structure models. In these models, occupancy factors of cations and anions are different. Model 3 gave the best results with lowest R factors.

	Site	Atom	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7	Model 8	Model 9
Occupancy factors	*A*	Y	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	1.000
		Ce	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.005	0.000
	B	Al	0.875	0.875	1.000	1.000	1.000	1.000	0.938	0.938	1.000
		Si	0.125	0.125	0.000	0.000	0.000	0.000	0.063	0.063	0.000
	C	Al	1.000	1.000	0.917	0.917	1.000	1.000	0.958	0.958	0.917
		Si	0.000	0.000	0.083	0.083	0.000	0.000	0.042	0.042	0.083
	X	O	0.979	1.000	0.979	1.000	0.979	1.000	0.979	1.000	0.979
		N	0.021	0.000	0.021	0.000	0.021	0.000	0.021	0.000	0.021
R_{wp} of TOF-NPD data	BS		0.0505	0.0502	0.0490	0.0502	0.0499	0.0495	0.0498	0.0502	0.0502
	90°		0.0419	0.0423	0.0413	0.0422	0.0418	0.0422	0.0417	0.0420	0.0418

The conditions of atom occupations of each model are as follows:

Model 1 (Ce at the *A* site, Si at the *B* site, and O and N at *X* site),

Model 2 (Ce at the *A* site, Si at the *B* site, and O at *X* site),

Model 3 (Ce at the *A* site, Si at the *C* site, and O and N at *X* site),

Model 4 (Ce at the *A* site, Si at the *C* site, and O at *X* site),

Model 5 (Ce at the *A* site, and O and N at *X* site),

Model 6 (Ce at the *A* site, and O at *X* site),

Model 7 (Ce at the *A* site, Si at 50% *B* and 50% *C* sites, and O and N at *X* site),

Model 8 (Ce at the *A* site, Si at 50% *B* and 50% *C* sites, and O at *X* site), and

Model 9 (Si at the *C* site, and O and N at *X* site).

PL and PLE spectra in YASiONG: Ce^{3+} phosphor

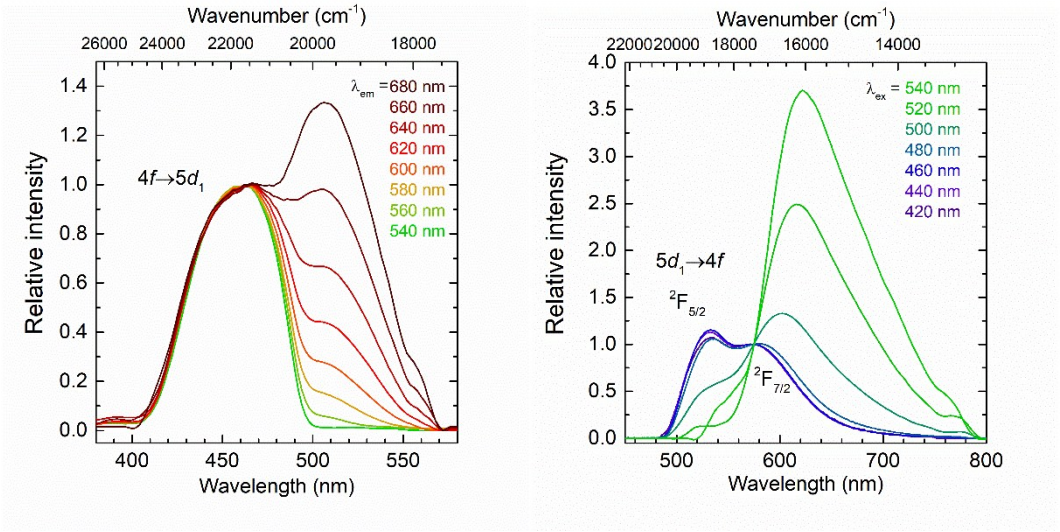

Fig. S3 (a) PLE and (b) PL spectra of YASiONG:Ce phosphor normalized at (a) 464nm (peak wavelength of $4f \rightarrow 5d_1$ transition) and (b)575 nm (peak wavelength of $5d_1 \rightarrow 4f\,(^2F_{7/2})$ transition)