Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

First-principles study of Ce-doped $Y_3Al_5O_{12}$ with Si–N incorporation: electronic structures and optical properties†

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Table S1 Calculated lattice parameters and volumes for YAG, YAG:Ce, YAG:$Si_{Al(tet)}$-N_O, and YAG:Ce,Si_{Ali}-N_{Oi} (i = 1, 2). In the last row, the percent changes of the 2nd and 3rd columns were taken with respect to the volume of YAG (1st Column), and the percent changes of the 4th and 5th columns were taken with respect to the volume of YAG:Ce (2nd column).

	YAG	YAG:Ce	YAG: $Si_{Al(tet)}$–N_O	YAG:Ce, Si_{Al1}–N_{O1}	YAG:Ce, Si_{Al2}–N_{O2}
a (Å)	12.000	12.016	11.986	11.999	12.022
b (Å)	12.000	12.007	11.994	12.014	12.004
c (Å)	12.000	12.007	11.970	12.005	11.990
α (deg)	90.000	90.056	90.077	89.998	90.059
β (deg)	90.000	90.000	90.000	89.976	89.917
γ (deg)	90.000	90.000	89.983	89.922	90.012
Volume (Å^3)	1728.000	1732.334	1720.816	1730.567	1730.387
		(+0.251%)	(−0.416%)	(−0.102%)	(−0.112%)

Fig. S1 Calculated total and orbital projected DOSs for YAG:Ce with the NN Si_{Al2}–N_{O2} substitution. The occupied Ce^{3+} 4f state is indicated by the dashed line, and its energy position with respect to the host VBM is indicated.