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Supporting Information

Green persistent luminescence and electronic structure of *β*-Sialon:Eu^{2+}

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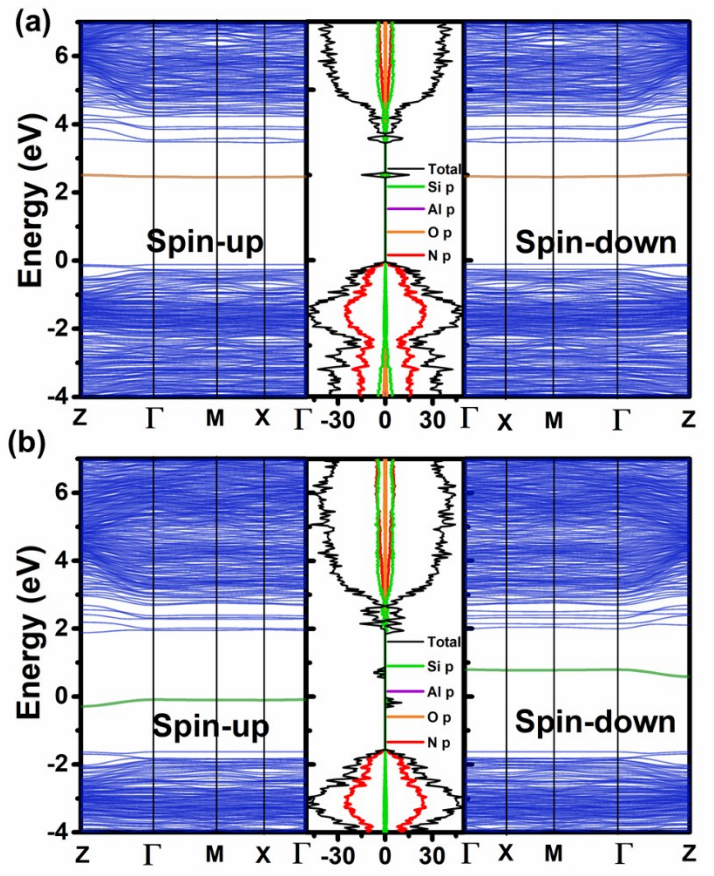

Fig. S1 Computed electronic band dispersion, DOS, and PDOS of the prefect compound β-Sialon (z = 0.5) with O vacancy (a), and N vacancy (b). In panel a, the impurity level of O vacancy is donated by brown line. The impurity level of N vacancy is donated by green line in panel b.

Table S1. Structural parameters of ESAON determined by Rietveld Refinement of Power XRD Data collected at room temperature.

Atom	Site	x	y	z	Occu	U(Å^2)
Si1	6h	0.1753(2)	0.7691(2)	0.2500(0)	0.921	1.0(7)
Al1	6h	0.1753(2)	0.7691(2)	0.2500(0)	0.079	1.5(8)
N1	6h	0.3316(4)	0.0297(4)	0.2500(0)	0.935	1.2(4)

O1	6h	0.3316(4)	0.0297(4)	0.2500(0)	0.065	1.2(4)
N2	2c	0.3333(0)	0.6667(0)	0.2500(0)	0.935	0.9(5)
O2	2c	0.3333(0)	0.6667(0)	0.2500(0)	0.065	0.9(5)
Eu1	2b	0.0000(0)	0.0000(0)	0.0000(0)	0.013	1.5(7)

Space group: $P6_3/m$ (No. 176), Z=2, V=146.2090(7), a=b=7.6131(2), c=2.9129(6), R_p=6.93%, R_{wp}=9.98%, χ^2=2.66

Table S2. Parameter value that determine the HRBE schemes of ESAON, including the energy for electrons in the 4*f* ground state of divalent $E_{vf}(Ln^{2+})$ and trivalent $E_{vf}(Ln^{3+})$ lanthanides, the energy for the lowest 5*d* state of divalent $E_{vd}(Ln^{2+})$ and trivalent $E_{vd}(Ln^{3+})$ lanthanides, the exciton energy (E_{ex}) and the band gap between the top of VB and the bottom of CB.

Ln	n	$E_{vf}(Ln^{2+})$ /eV	$E_{vf}(Ln^{3+})$ /eV	$E_{vd}(Ln^{2+})$ /eV	$E_{vd}(Ln^{3+})$ /eV
La	0	8.76	—	6.27	—
Ce	1	7.28	2.08	6.11	5.41
Pr	2	6.02	0.23	6.06	5.07
Nd	3	5.67	-1.26	5.99	4.87
Pm	4	5.49	-1.70	5.90	4.75
Sm	5	4.40	-1.89	5.85	4.66
Eu	6	3.15	-3.16	5.82	4.93
Gd	7	7.71	-4.50	5.96	4.51
Tb	8	6.36	0.41	6.00	5.40
Dy	9	5.42	-1.01	6.04	5.45
Ho	10	5.15	-2.11	5.85	5.20
Er	11	5.73	-2.04	6.30	5.03
Tm	12	4.87	-1.88	6.27	5.08
Yb	13	3.58	-2.92	6.25	5.15
Lu	14	—	-4.17	—	5.30

E^{ex}: 6.30 eV; Band gap: 6.80 eV