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SUPPORTING INFORMATION

Red persistent and photostimulable phosphor $SrLiAl_3N_4$: Eu^{2+}

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Table S1. Main parameters of processing and refinement of the $SrLiAl_3N_4$ (SLAN) samples.

Compound	$SrLiAl_3N_4$
Space Group	*P*-3*m*1
a, Å	5.855 (1)
b, Å	7.483 (4)
c, Å	9.932 (2)
α, Å	83.61 (9)
β, Å	76.76 (7)
γ, Å	79.54 (9)
V, Å^3	415.50 (1)
R_p, %	14.0
R_{wp}, %	14.1
R_{exp}, %	8.59
χ^2	1.64

Table S2. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of SLAN.

Atom	*x*	*y*	*z*	B_{iso}	Occ.
Sr1	0.001 (7)	0.131 (7)	0.124 (3)	0.114 (6)	1
Sr2	0.020 (4)	0.382 (5)	0.375 (1)	0.077 (9)	1
Al1	0.537 (1)	0.955 (3)	0.127 (8)	0.299 (5)	1
Al2	0.172 (1)	0.957 (5)	0.388 (8)	0.000 (0)	1
Al3	0.169 (8)	0.703 (4)	0.155 (2)	0.000 (0)	1

Al4	0.814 (8)	0.563 (0)	0.107 (7)	0.713 (2)	1
Al5	0.468 (8)	0.564 (8)	0.373 (5)	0.681 (5)	1
Al6	0.571 (2)	0.190 (4)	0.362 (6)	0.000 (0)	1
N1	0.374 (7)	0.854 (7)	0.005 (3)	0.000 (0)	1
N2	0.388 (5)	0.357 (2)	0.512 (9)	0.000 (0)	1
N3	0.372 (4)	0.111 (4)	0.276 (3)	0.943 (7)	1
N4	0.156 (9)	0.939 (9)	0.597 (0)	0.000 (0)	1
N5	0.843 (2)	0.775 (3)	0.160 (5)	0.252 (2)	1
N6	0.240 (2)	0.459 (2)	0.089 (0)	0.000 (0)	1
N7	0.203 (1)	0.705 (6)	0.349 (7)	0.000 (0)	1
N8	0.671 (4)	0.386 (9)	0.246 (2)	0.000 (0)	1
Li1	0.482 (8)	0.282 (6)	0.147 (6)	0.000 (0)	1
Li2	0.223 (2)	0.180 (8)	0.656 (7)	0.000 (0)	1

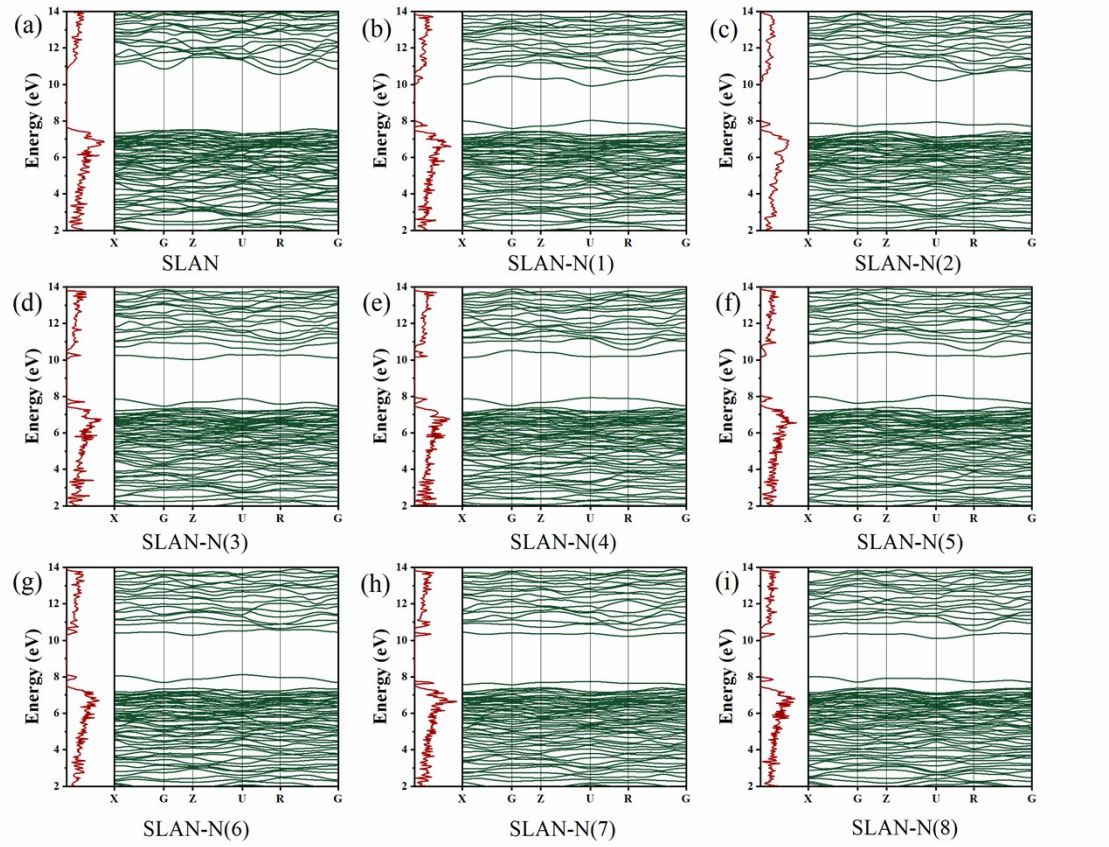

Fig. S1. DOS and computed electronic band dispersion of (a) the perfect compound SLAN and (b) SLAN with $V_{N(1)}$ (c) $V_{N(2)}$ (d) $V_{N(3)}$ (e) $V_{N(4)}$ (f) $V_{N(5)}$ (g) $V_{N(6)}$ (h) $V_{N(7)}$ (i) $V_{N(8)}$

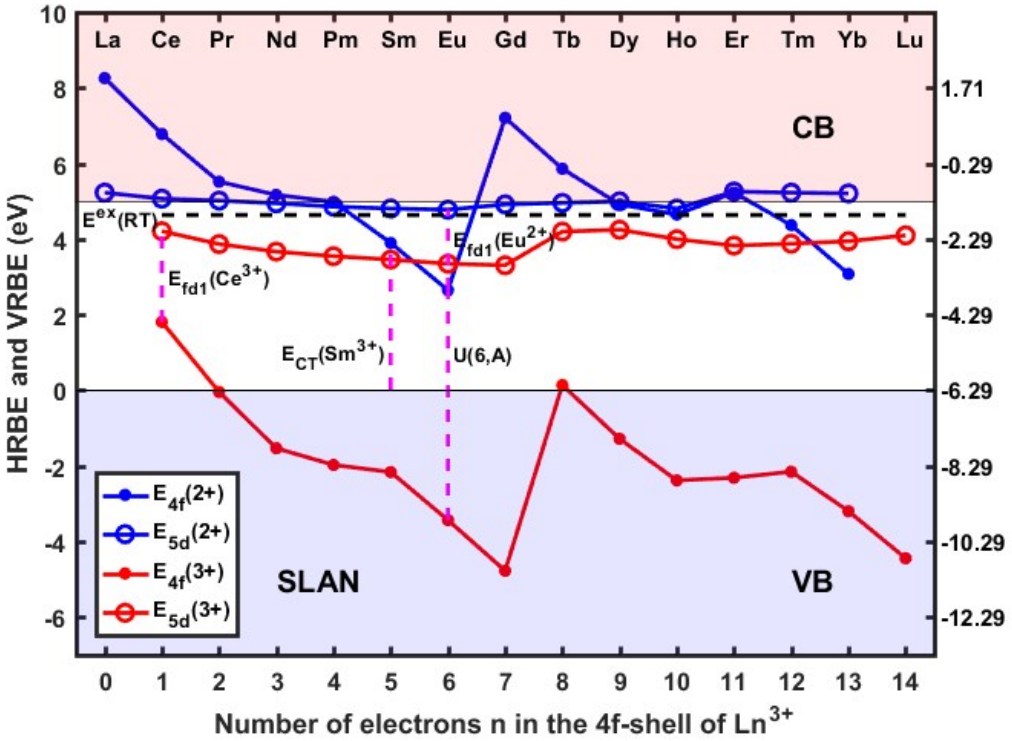

Fig. S2. HRBE and VRBE diagram of SLAN

Table S3. Parameter value that determine the HRBE schemes of SLAN, including the energy for electrons in the 4f-ground state of divalent $E_{4f}(Ln^{2+})$ and trivalent $E_{4f}(Ln^{3+})$, the energy for the lowest 5d state of divalent $E_{5d}(Ln^{2+})$ and trivalent $E_{5d}(Ln^{3+})$ lanthanides and the band gap between the top of valence band and the bottom of conduction band (E_{VC}).

Ln	n	$E_{4f}(Ln^{2+})$/eV	$E_{4f}(Ln^{3+})$/eV	$E_{5d}(Ln^{2+})$/eV	$E_{5d}(Ln^{3+})$/eV
La	0	8.26		5.23	
Ce	1	6.78	1.81	5.07	4.21
Pr	2	5.52	-0.04	5.02	3.87
Nd	3	5.17	-1.53	4.95	3.67
Pm	4	4.99	-1.97	4.86	3.55
Sm	5	3.90	-2.16	4.81	3.46
Eu	6	2.65	-3.43	4.78	3.35
Gd	7	7.21	-4.77	4.92	3.31
Tb	8	5.86	0.14	4.96	4.20
Dy	9	4.92	-1.28	5.00	4.25
Ho	10	4.65	-2.38	4.81	4.00
Er	11	5.23	-2.31	5.26	3.83
Tm	12	4.37	-2.15	5.23	3.88

Yb	13	3.08	-3.19	5.21	3.95
Lu	14		-4.44		4.10

E_{VC} = 4.96 eV