Supporting Information

Stimulated-source-independent Persistent Luminescence Phosphor $Sr_2Ta_2O_7:Tb^{3+}$, Tm^{3+} for Multi-mode Anti-counterfeiting Applications

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Occupied sites	R_{host} **(Å)**	R_{atom} **(Å)**	ΔR **(%)**
Tb → Sr	1.18	0.92	22.03
Tb → Ta	0.64	0.92	43.75
Tm → Sr	1.18	0.88	25.42
Tm → Ta	0.64	0.88	37.50

Table S1 Ions radius difference between cations of host and Tb^{3+}/Tm^{3+}(CN=6).

Occupied sites	E_T (doped) (eV)	E_T (bulk) (eV)	E_{atom} (eV)	E_{dopant} (eV)	E_{form} (eV)
Tb → Sr1	-193.45	-190.62	-1.63	-4.55	-0.14
Tb → Sr2	-192.60	-190.62	-1.63	-4.55	0.94
Tb → Ta	-178.42	-190.62	-11.81	-4.55	4.94
Tm → Sr1	-193.22	-190.62	-1.63	-4.45	0.21
Tm → Sr2	-192.19	-190.62	-1.63	-4.45	1.24
Tm → Ta	-179.02	-190.62	-11.81	-4.45	4.23

Table S2 Formation energy as Tb^{3+}/Tm^{3+} occupy different cations in STO.

doped ions	Bond length 1 (Å)	Bond length 2 (Å)	Bond length 3 (Å)	Bond length 4 (Å)	Bond length 5 (Å)	Bond length 6 (Å)	Average bond length (Å)	Distortion (Δd)
Tb	2.3069	2.3069	2.3069	2.3069	2.2769	2.2769	2.2969	3.0625
Tb, Tm	2.3383	2.3383	2.3383	2.3383	2.2820	2.2820	2.3195	5.7968

Table S3 Different co-doped ions lead to distortion degree comparison of Tb^{3+} sites.

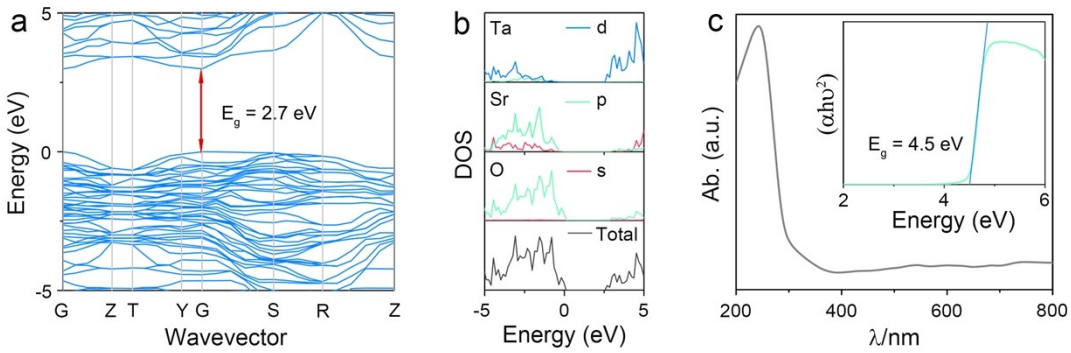

Fig. S1 (a) The band structure, (b) PDOS and (c) the absorption spectrum as well as the Taucc curve of STO.

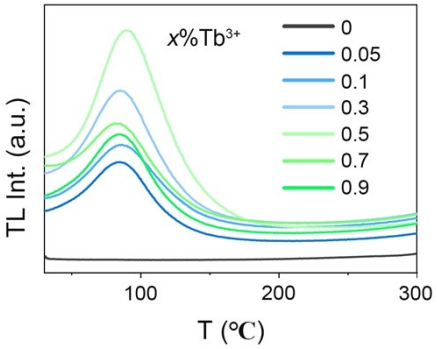

Fig. S2 The TL curves of STO:x%Tb^{3+} (x = 0, 0.05, 0.1, 0.3, 0.5, 0.7, 0.9).

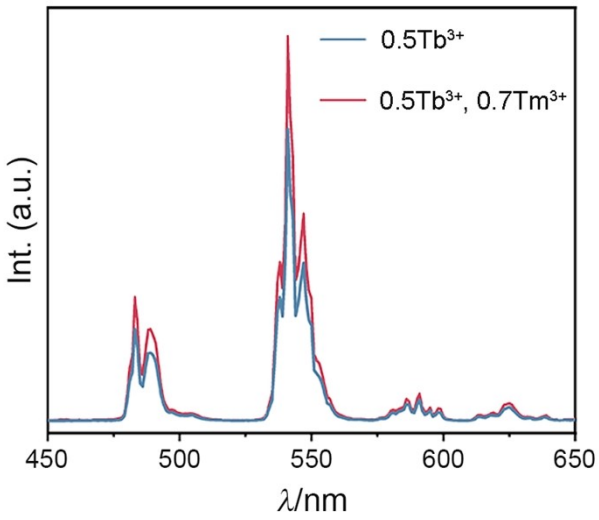

Fig. S3 PL spectra of STO:0.5%Tb^{3+} and STO:0.5%Tb^{3+},0.7%Tm^{3+} phosphors under the excitation of 262 nm.

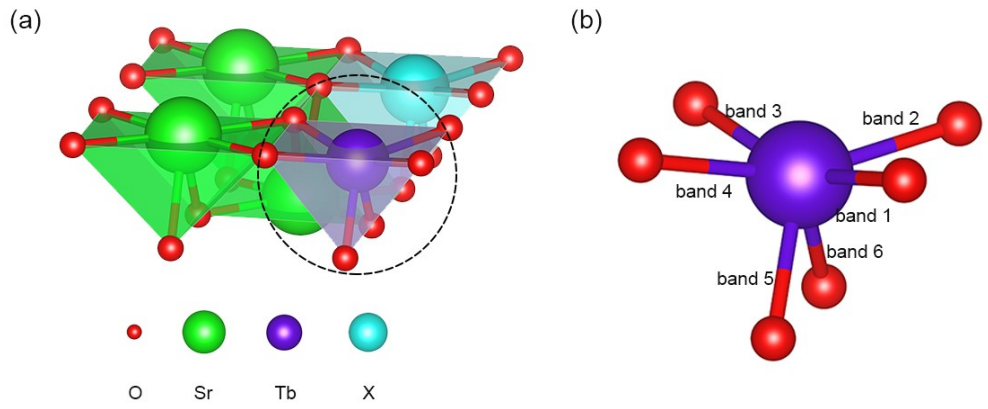

Fig. S4 (a) Enlarged view of STO crystal structure (X=Tm, Sr). (b) Enlarged view of Tb occupied site.

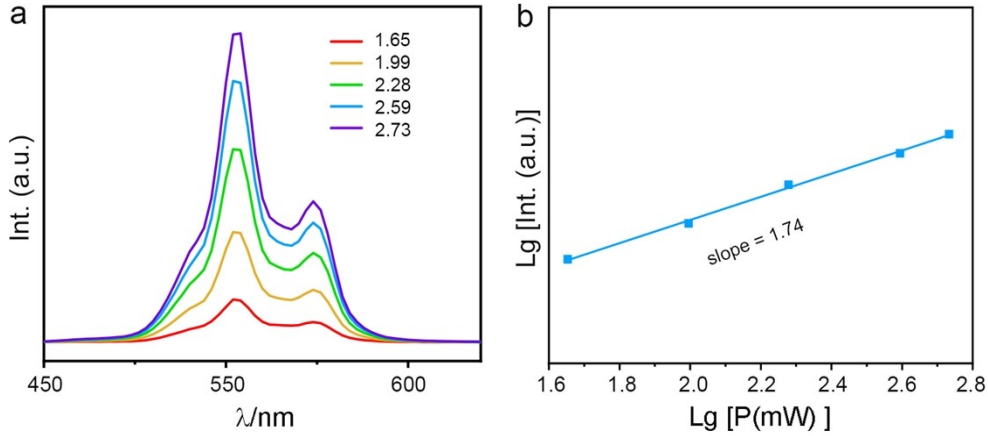

Fig. S5 (a)The PL spectra under variable excitation power of 808 nm NIR laser. (b) Dual logarithmic plots of UC emission intensity *versus* pumping power of STO: Tb^{3+}, Tm^{3+}.