Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Enhancing the Inherent NIR Photoluminescence in $SrLaLiTeO_6$ Through Cr^{3+}-Yb^{3+} Co-substitution for High Performance pc-LEDs

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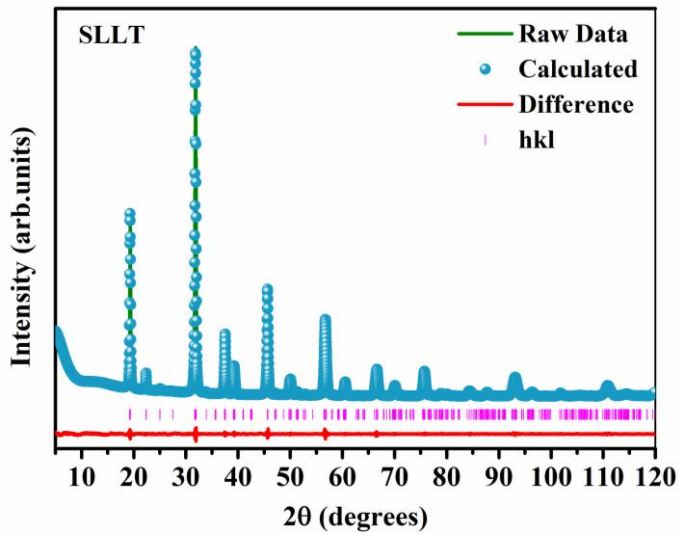

Figure S1. Rietveld refinement of XRD pattern of SLLT.

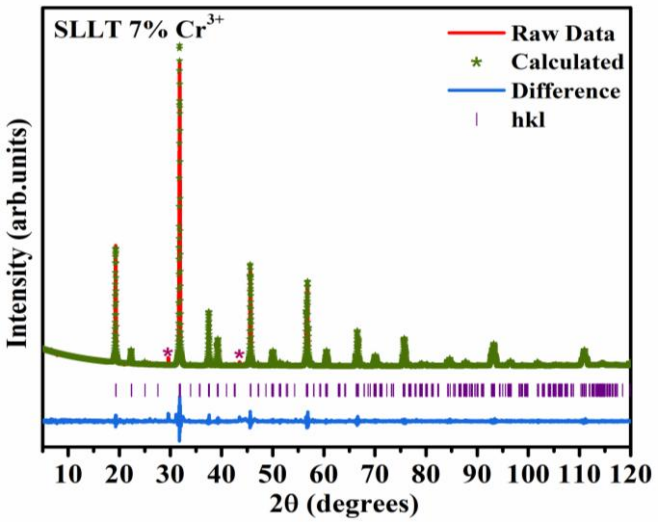

Figure S2. Le Bail fit of XRD patterns of SLLT: 7% Cr^{3+}.

Table S1. Lattice Parameters of SLLT x%Cr^{3+} (x =0, 0.5, 0.7, 1, 3, 7 and 10 mol%).

Double Perovskites	a (Å)	b (Å)	c (Å)	β (˚)
SLLT	5.64(4)	5.59 (8)	7.93(2)	90.22(1)
SLLT: 0.5% Cr^{3+}	5.63(1)	5.59 (8)	7.93(1)	90.05(5)
SLLT: 0.7% Cr^{3+}	5.63(1)	5.59(7)	7.93(1)	90.05(5)
SLLT: 1% Cr^{3+}	5.63(1)	5.59(8)	7.93(1)	90.05(5)
SLLT: 3% Cr^{3+}	5.63(2)	5.59(9)	7.93(1)	90.05(9)
SLLT: 7% Cr^{3+}	5.63(1)	5.59(8)	7.92(9)	90.05(5)
SLLT: 10% Cr^{3+}	5.63(1)	5.59(1)	7.93(1)	90.05(5)

Table S2. Refined crystallographic parameters of SLLT:3% Cr^{3+}.

Atom	Site	x	y	z	Occupancy	B_{eq} (Å^2)
Sr	*4e*	0.492 (6)	0.552 (7)	0.252 (3)	0.5	1.26 (9)
La	*4e*	0.492 (6)	0.552 (7)	0.252(3)	0.5	1.26 (9)
Li	*2c*	0.5	0	0	1	0.25(9)
Cr1	*2c*	0.5	0	0	1	0.26 (1)
Te	*2d*	0	0.5	0	1	0.23 (2)
Cr2	*2d*	0	0.5	0	1	0.26 (1)
O1	*4e*	0.217 (3)	0.241 (1)	0.050 (9)	1	2.35(2)
O2	*4e*	0.205 (1)	0.775 (9)	0.024(9)	1	2.55(2)
O3	*4e*	0.533 (9)	0.020 (9)	0.258 (9)	1	2.55(2)

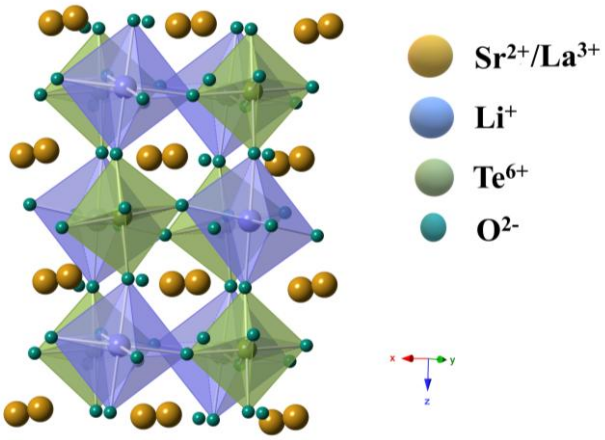

Figure S3. Crystal structure of SLLT.

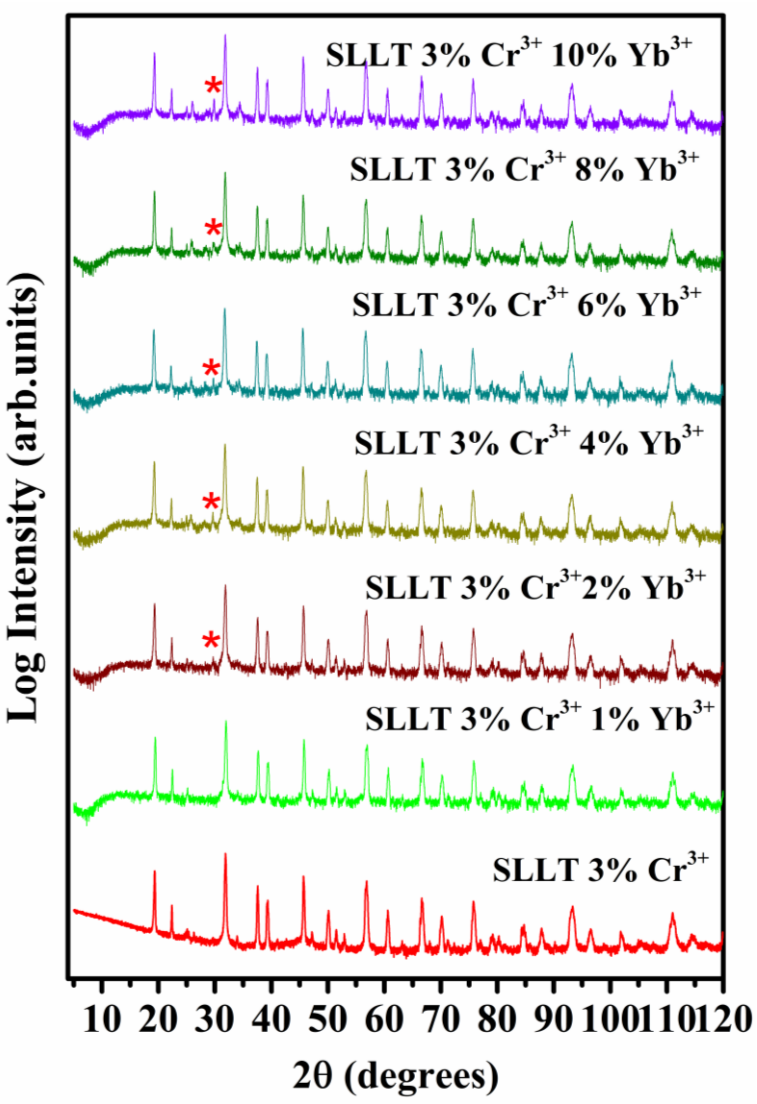

Figure S4. XRD patterns of SLLT:3%Cr^{3+}, y% Yb^{3+} (y =0, 1, 2, 4, 6, 8 and 10 mol%).

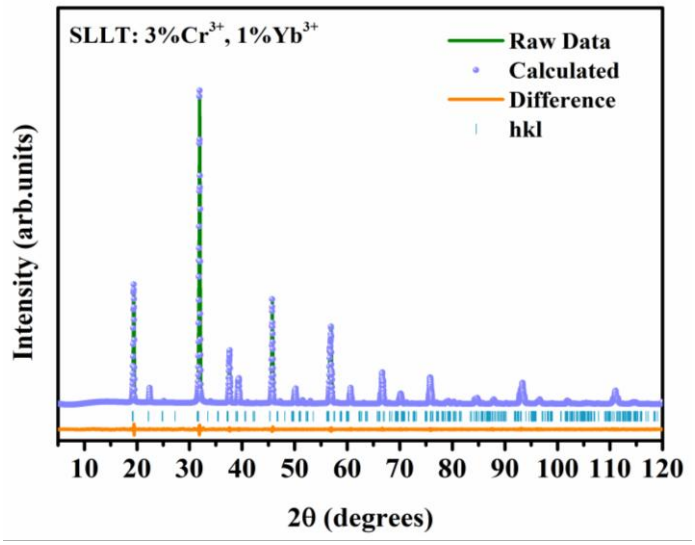

Figure S5. Rietveld refinement of XRD pattern of SLLT:3%Cr^{3+}, 1% Yb^{3+}.

Table S3. Refined crystallographic parameters of SLLT: 3% Cr^{3+},1% Yb^{3+}.

Atom	Site	x	y	z	Occupancy	B_{eq} (Å^2)
Sr	*4e*	0.559 (1)	0.468 (5)	0.242 (5)	0.5	1.30 (9)
La	*4e*	0.559 (1)	0.468 (5)	0.242 (5)	0.5	1.30 (9)
Yb	*4e*	0.559 (1)	0.468 (5)	0.242 (5)	0.5	1.30(9)
Li	*2c*	0.5	0	0	1	0.20(9)
Cr1	*2c*	0.5	0	0	1	0.20 (9)
Te	*2d*	0	0.5	0	1	0.23 (1)
Cr2	*2d*	0	0.5	0	1	0.30 (1)
O1	*4e*	0.217 (3)	0.241 (1)	0.050 (9)	1	2.30(1)
O2	*4e*	0.205 (1)	0.775 (9)	0.024(9)	1	2.50(1)
O3	*4e*	0.533 (9)	0.020 (9)	0.258 (9)	1	2.50(1)

Table S4. Rietveld refinement parameters of SLLT, SLLT: 3% Cr^{3+}, and SLLT:3% Cr^{3+},1% Yb^{3+}.

Compound	a (Å)	b (Å)	c (Å)	β°	R_{exp}	R_{wp}	R_p	χ^2	Ref.
SLLT	5.6443(9)	5.5982(3)	7.9321(9)	90.220 (6)	2.07	3.71	2.82	1.79	(i)
SLLT: 3% Cr^{3+}	5.6189 (3)	5.6205(3)	7.9687 (9)	90.28°	5.44	5.94	4.15	1.09	This work
SLLT:3% Cr^{3+}, 1% Yb^{3+}	5.6089 (5)	5.5927(7)	7.9429 (5)	90.32°	2.85	4.06	2.92	1.42	This work

References

(i) B. Amrithakrishnan and G. Subodh, *Mater. Res. Bull.*, 2017, **93**, 177–182.

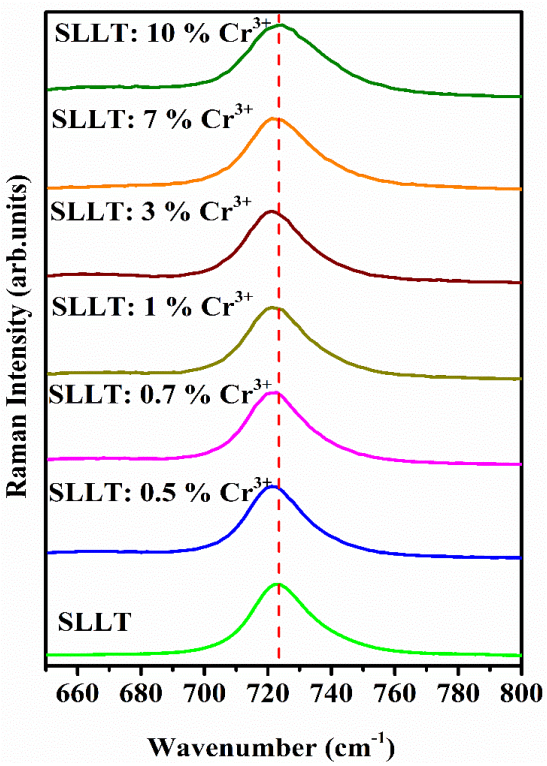

Figure S6. Redshift of Raman mode centered at 724 cm^{-1} corresponds to the symmetric stretching vibration of the TeO_6 octahedron.

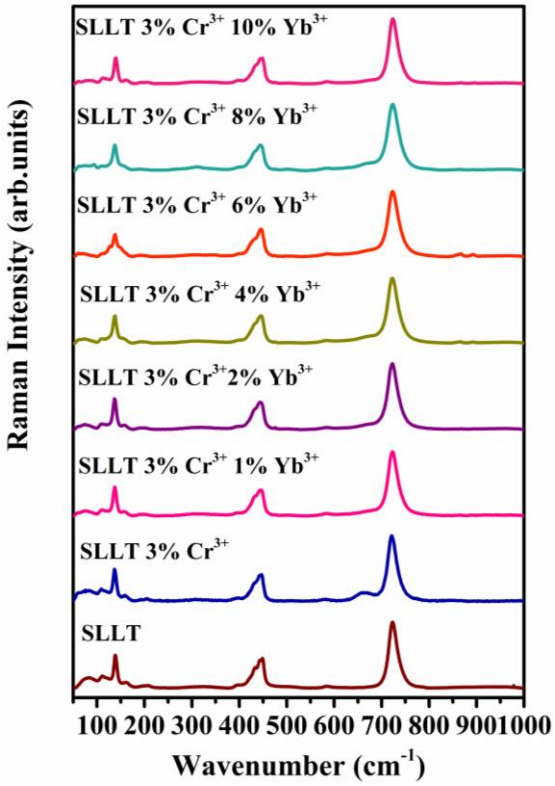

Figure S7. Raman spectra of SLLT and SLLT:3%Cr^{3+}, y% Yb^{3+} (x =0, 1, 2, 4, 6, 8 and 10 mol%).

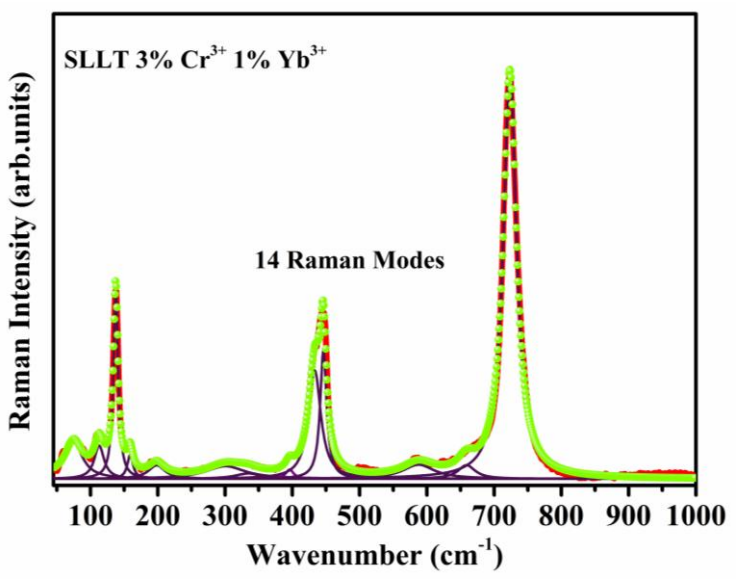

Figure S8: Deconvoluted Raman spectra of SLLT:3% Cr^{3+}, 1% Yb^{3+}.

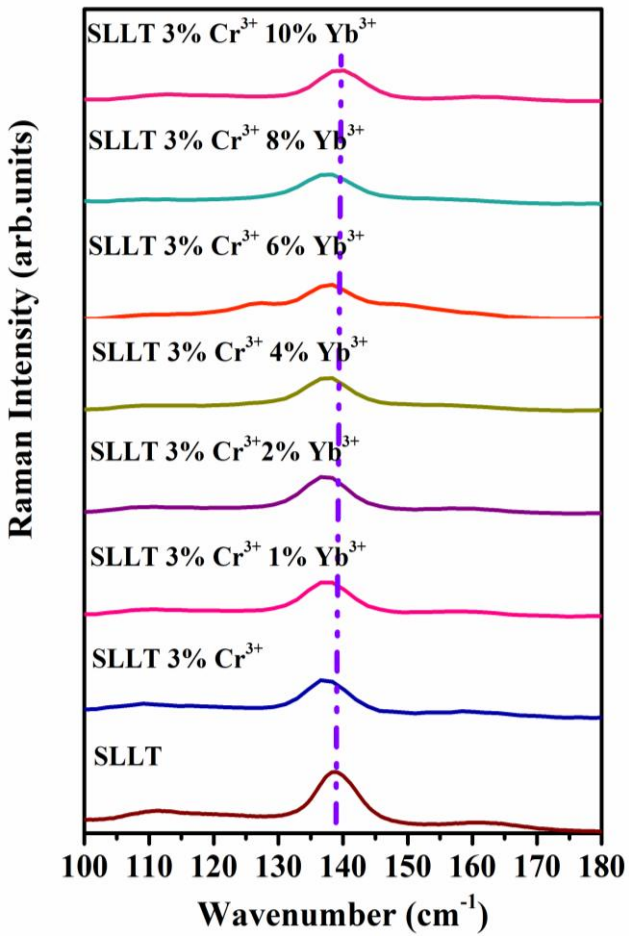

Figure S9. Redshift of Raman mode centered at 138 cm^{-1} corresponds to the translational modes of the A-site cations.

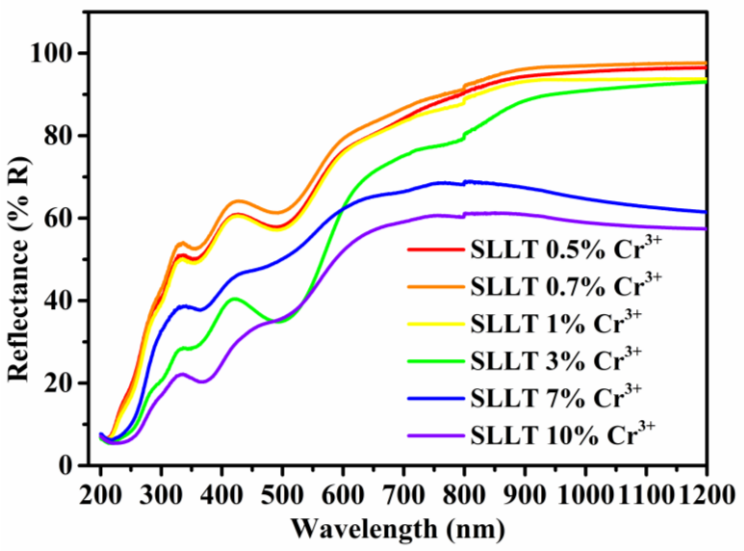

Figure S10. DRS of SLLT: x% Cr^{3+} (x = 0, 0.5, 0.7, 1, 3, 7 and 10 mol%).

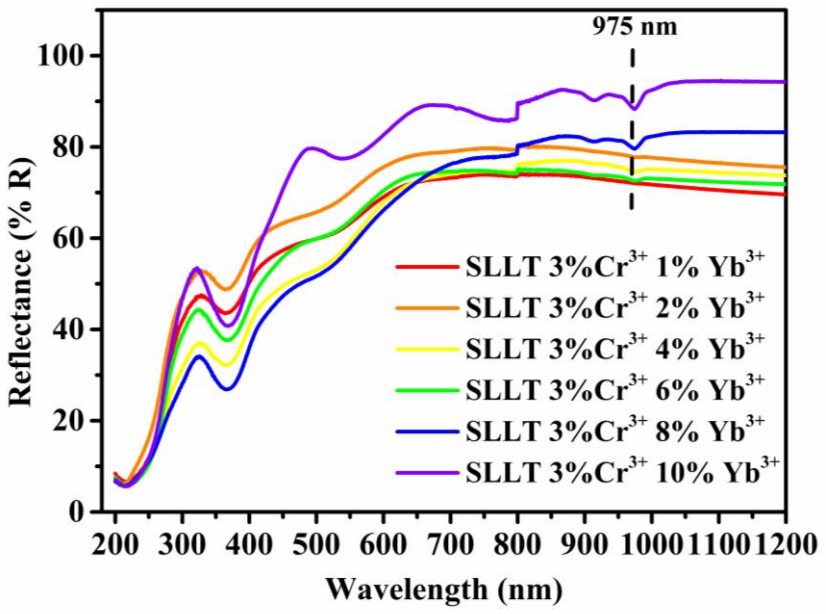

Figure S11. DRS of SLLT: 3% Cr^{3+}, y% Yb^{3+} (y = 1, 2, 4, 6, 8, and 10 mol%).

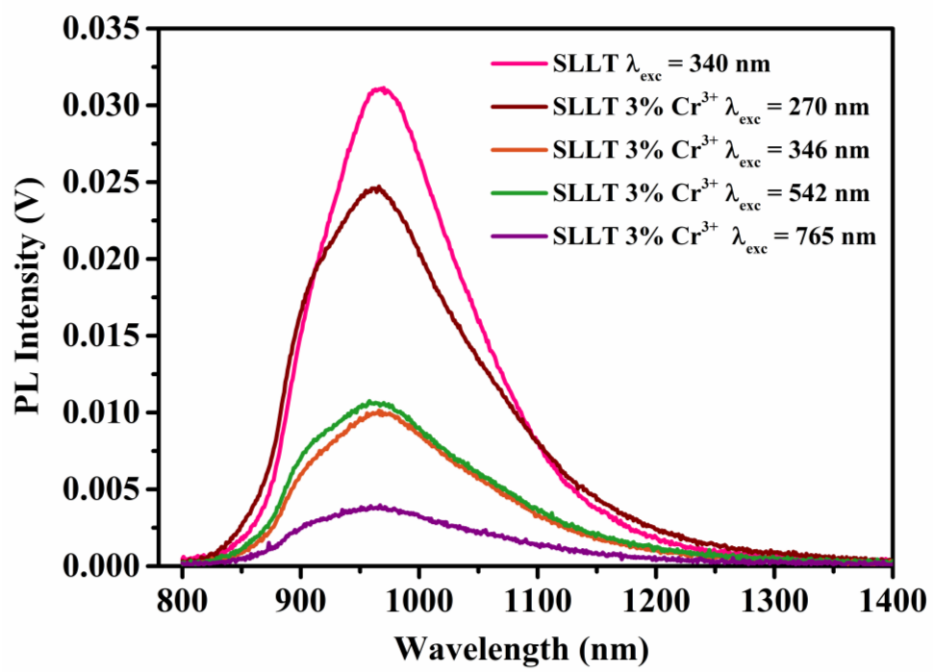

Figure S12. PL spectra of SLLT: 3% Cr^{3+} under different excitations.

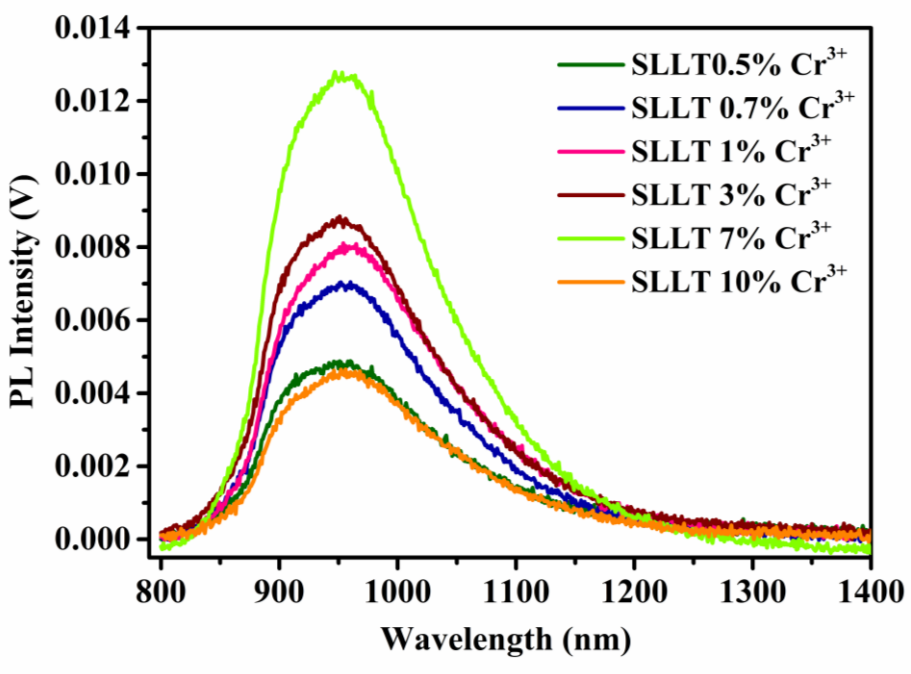

Figure S13. Concentration-dependent PL of SLLT: x%Cr^{3+} (x =0, 0.5, 0.7, 1, 3, 7 and 10 mol%).

Table S5. PL Lifetime of SLLT: x%Cr^{3+} (x = 0, 0.5, 0.7, 1, 3, 7 and 10 mol%)**.**

Double Perovskites	τ_{avg} (µs)
SLLT	333 ±1.11
SLLT: 0.5% Cr^{3+}	36 ± 1.35
SLLT: 0.7% Cr^{3+}	36 ± 1.55
SLLT: 1% Cr^{3+}	32 ± 1.38
SLLT: 3% Cr^{3+}	29 ± 1.39
SLLT: 7% Cr^{3+}	27 ± 1.89
SLLT: 10% Cr^{3+}	26 ± 1.54

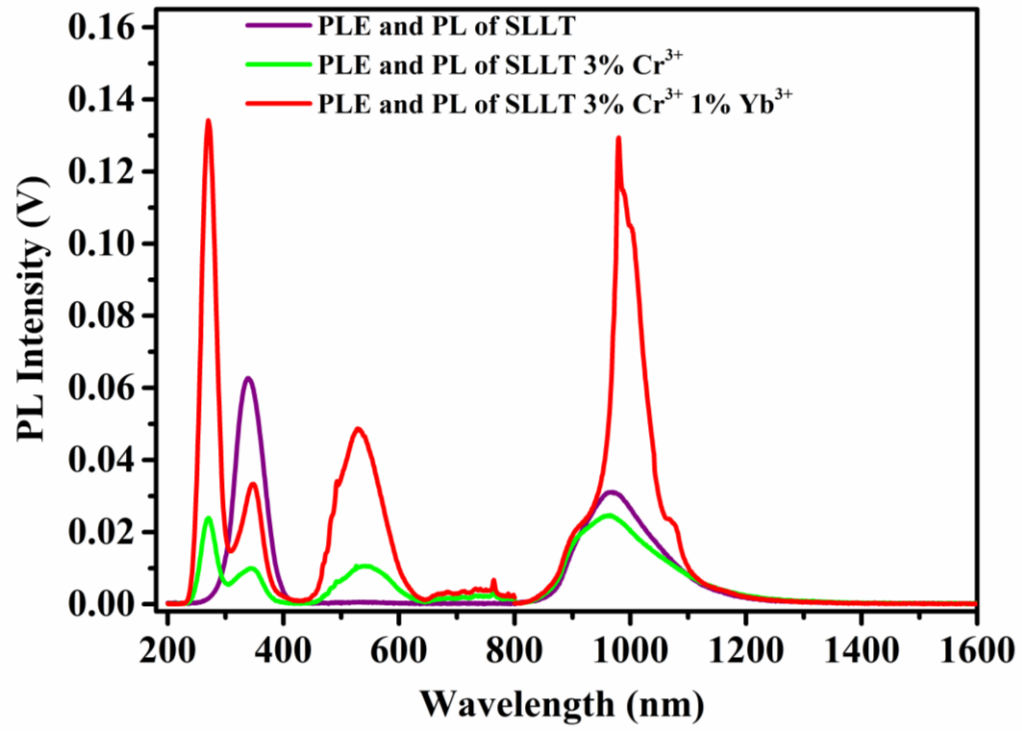

Figure S14. PLE and PL spectra of SLLT, SLLT: 3% Cr^{3+}, and SLLT: 3% Cr^{3+},1% Yb^{3+}.

Table S6. Energy transfer efficiencies of SLLT: 3% Cr^{3+}, y% Yb^{3+} (y = 1, 2, 4, 6, 8 and 10 mol%)

Double Perovskites	η (%)
SLLT: 3% Cr^{3+}, 1% Yb^{3+}	21
SLLT: 3% Cr^{3+}, 2% Yb^{3+}	21
SLLT: 3% Cr^{3+}, 4% Yb^{3+}	37
SLLT: 3% Cr^{3+}, 6% Yb^{3+}	39
SLLT: 3% Cr^{3+}, 8% Yb^{3+}	55
SLLT: 3% Cr^{3+}, 10% Yb^{3+}	59

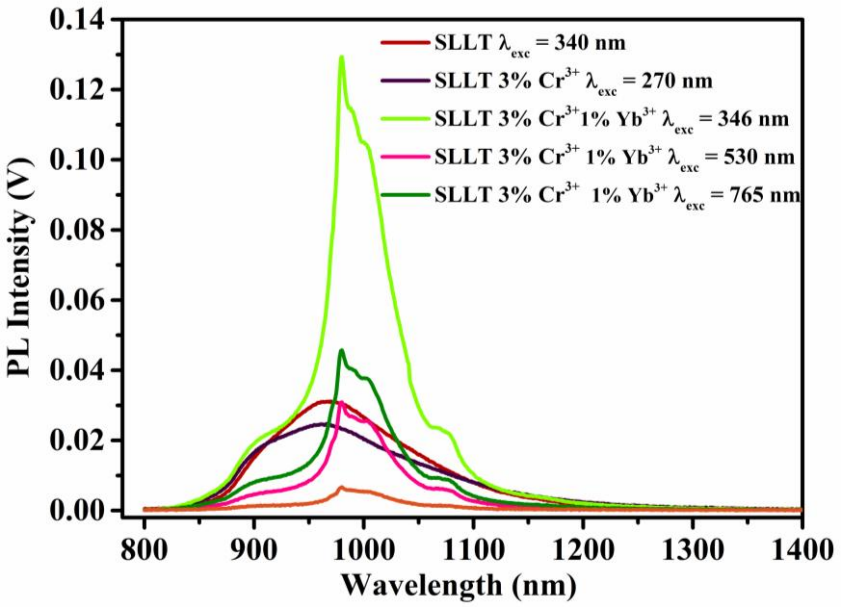

Figure S15. PL spectra of SLLT: 3% Cr^{3+}, 1% Yb^{3+} under different excitations.

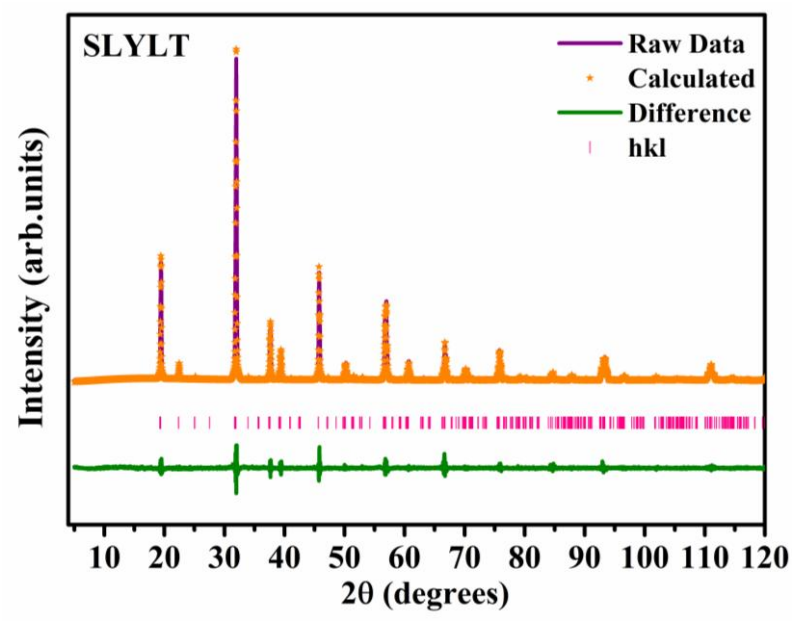

Figure S16. Le Bail fit of XRD pattern of SLLT: 1% Yb^{3+}.

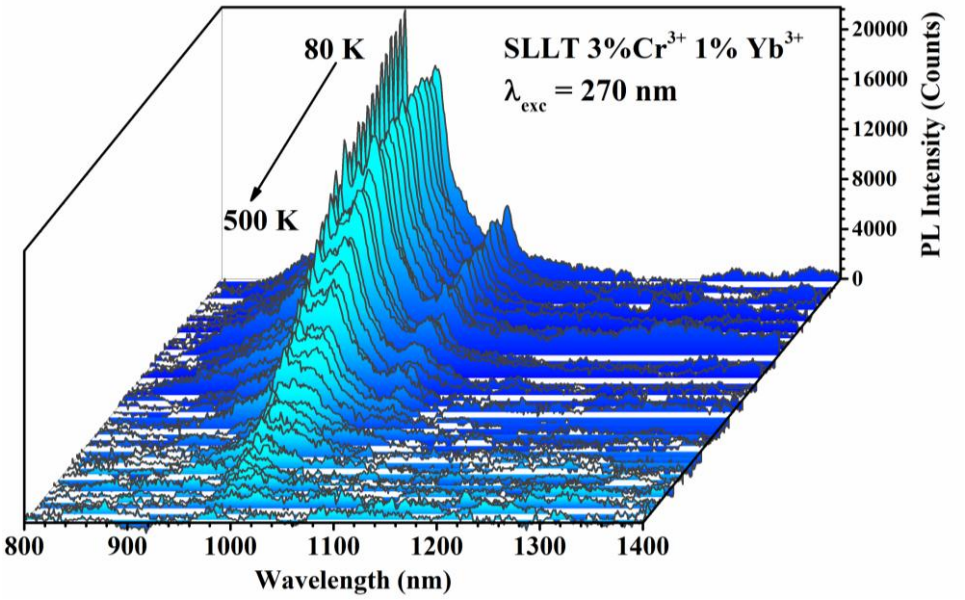

Figure S17. Temperature-dependent PL spectra of SLLT: 3% Cr^{3+}, 1% Yb^{3+}.

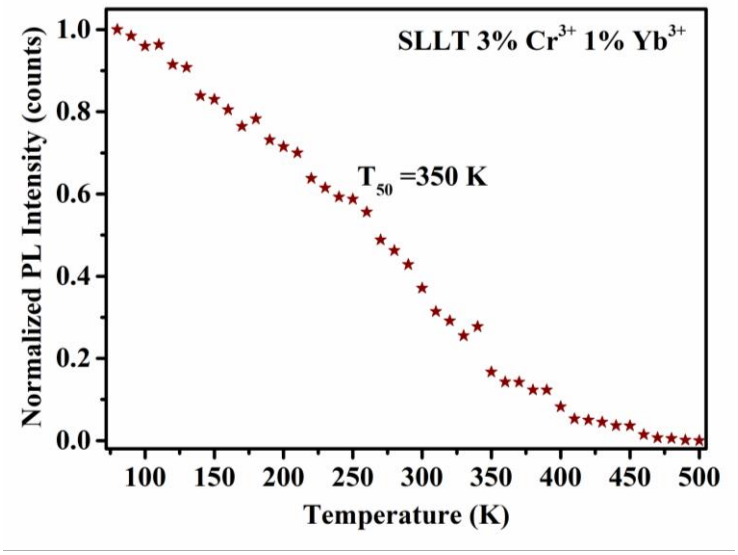

Figure S18. Temperature *vs* PL intensity plot of SLLT: 3% Cr^{3+}, 1% Yb^{3+}.

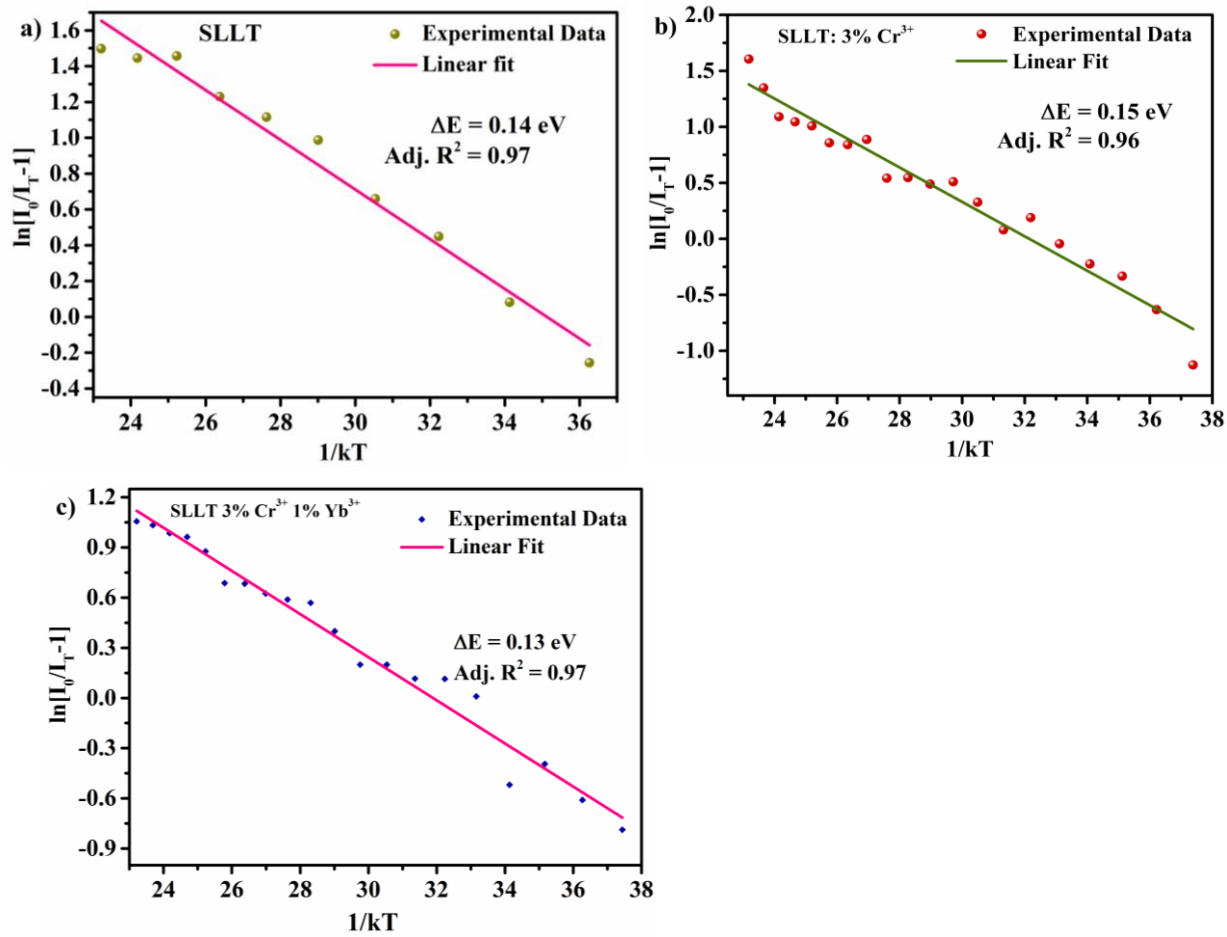

Figure S19. Plot of 1/kT *vs* $\ln(I_0/I_T-1)$ of **(a)** SLLT **(b)** SLLT: 3%Cr^{3+}, and **(c)** SLLT: 3%Cr^{3+}, 1% Yb^{3+}.

Table S7. Comparison of phosphor parameters of Cr^{3+} activated double perovskites.

Phosphor	Emission band (nm)	Activation energy, ΔE (eV)	Crystal field strength, D_q/B (cm^{-1})	B/B_0	Ref.
$La_2MgZrO_6:Cr^{3+}$	650-1250	0.089	2.49	0.674	[1]
$Ca_2GaNbO_6:Cr^{3+}$	680-840	-	2.31	0.57	[2]
$Ca_2AlNbO_6: Cr^{3+}$	680-840	-	2.65	0.53	[2]
$La_2ZnTiO_6:Cr^{3+}$	675-875	0.36	2.33	0.77	[3]
$Sr_2MgWO_6:Cr^{3+}$	675-1025	-	2.924	0.45	[4]
$Ba_2LaNbO_6:Cr^{3+}$	720-760	-	-	-	[5]
$Ca_2MgWO_6:Cr^{3+}$	700-1050	-	2.006	-	[6]
$La_2MgGeO_6:Cr^{3+}$	650-750	-	3.01	-	[7]
$Sr_2ScSbO_6: Cr^{3+}$	775-1075	-	2.03	0.51	[8]
$SrLaLiTeO_6:Cr^{3+}$	800-1225	0.15	2.28	0.48	This work

References

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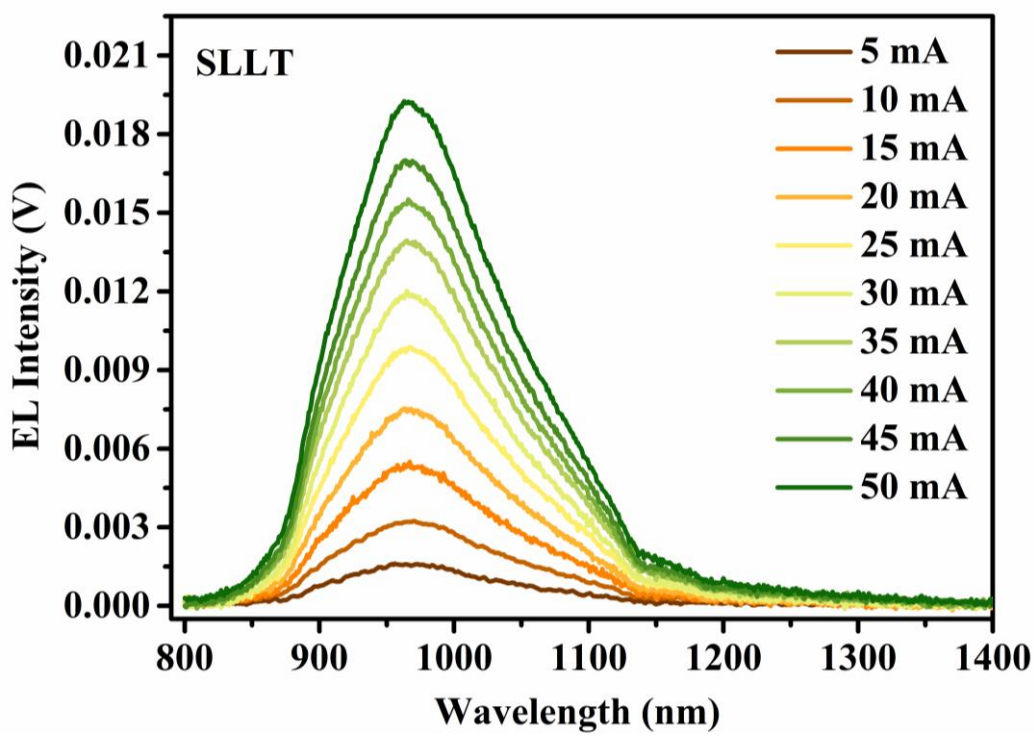

Figure S20. Electroluminescence spectra of SLLT.

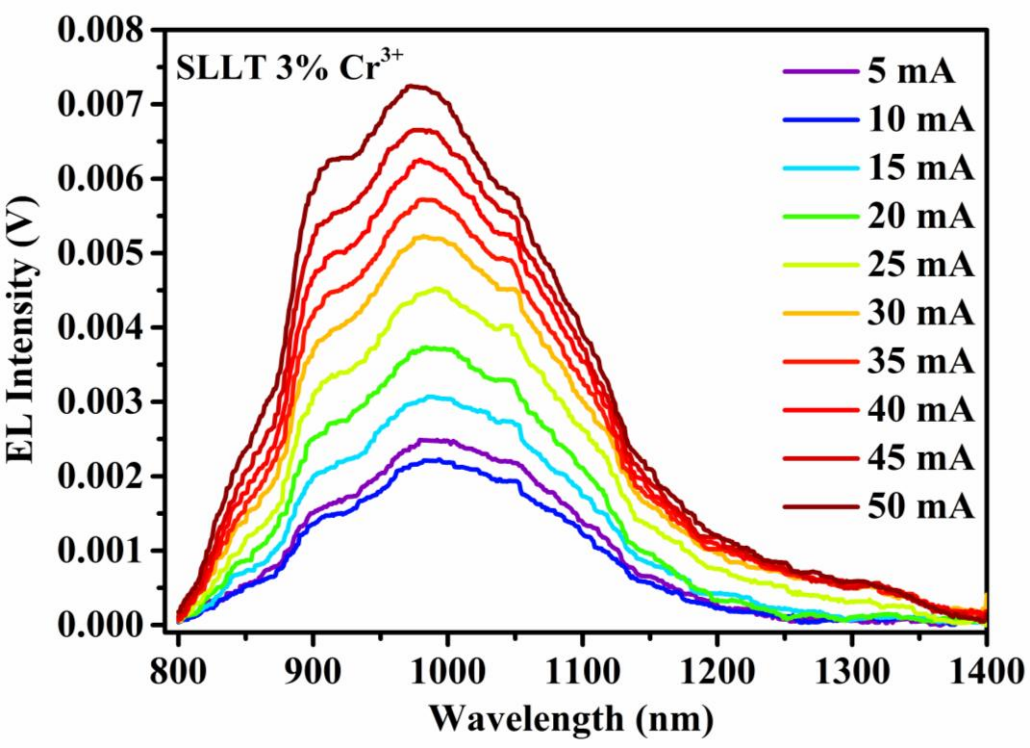

Figure S21. Electroluminescence spectra of SLLT: 3% Cr^{3+}.