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

Sb^{3+}/Mn^{2+} co-doped lead-free Cs_2KYCl_6 perovskites for white light-emitting diodes

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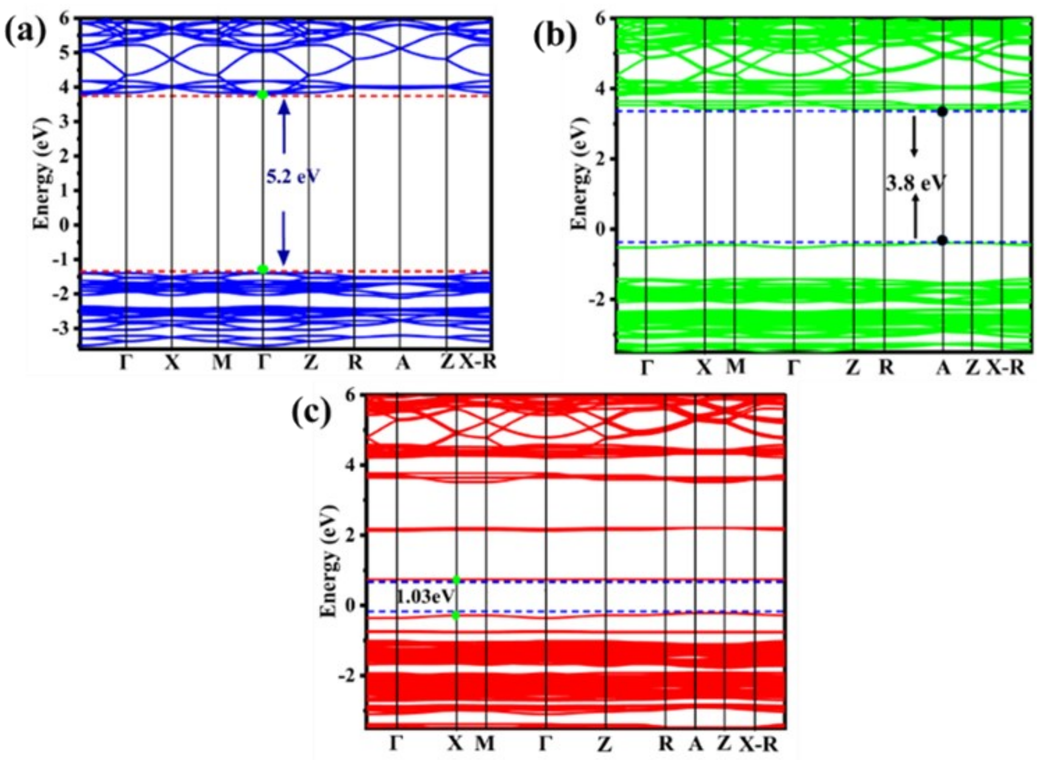

Fig.S1 Calculated band gaps for (a) Pristine Cs_2KYCl_6 MCs (b) Sb^{3+}-doped Cs_2KYCl_6 (c) and Sb^{3+}/Mn^{2+} co-doped Cs_2KYCl_6 MCs.

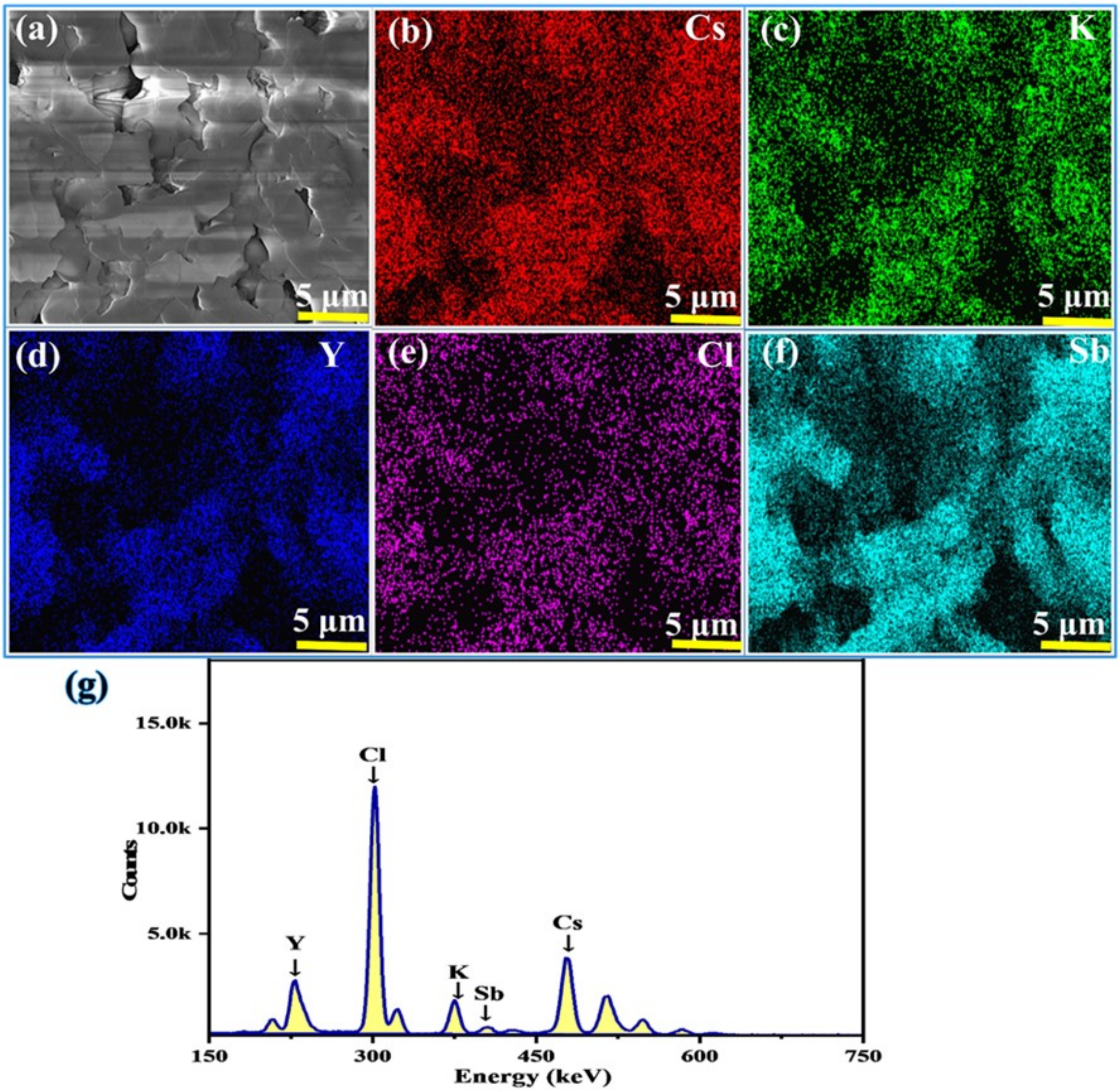

Fig. S2 (a) SEM image (b-f) mapping images of Sb^{3+} -doped Cs_2KYCl_6 (g) EDX spectrum.

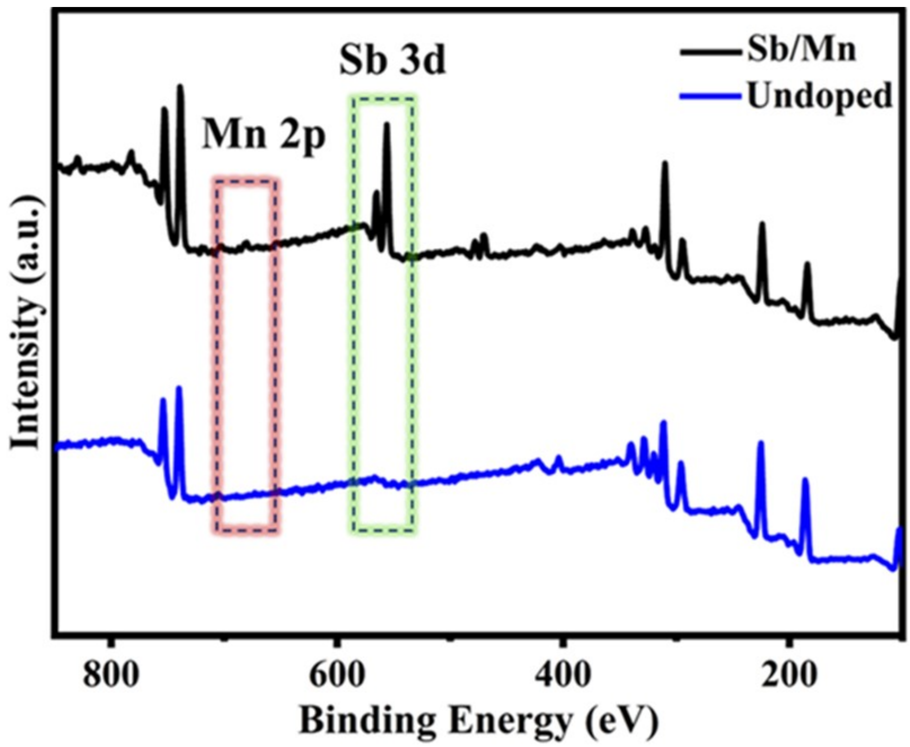

Fig. S3 (a) XPS survey spectra of pristine and Sb^{3+}/Mn^{2+} co-doped C_2KYCl_6 MCs.

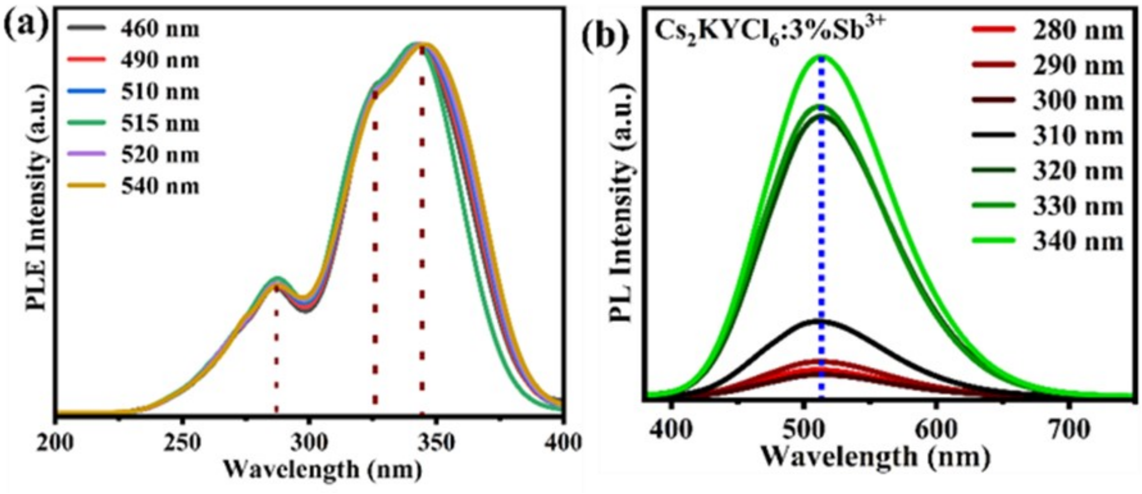

Fig. S4 (a) Normalized PLE spectra of 3% Sb^{3+} single-doped Cs_2KYCl_6 under different emission wavelengths (460 nm, 490 nm, 510 nm, 515 nm, 520 nm, and 540 nm). (b) PL spectra of Cs_2KYCl_6:3% Sb^{3+}.

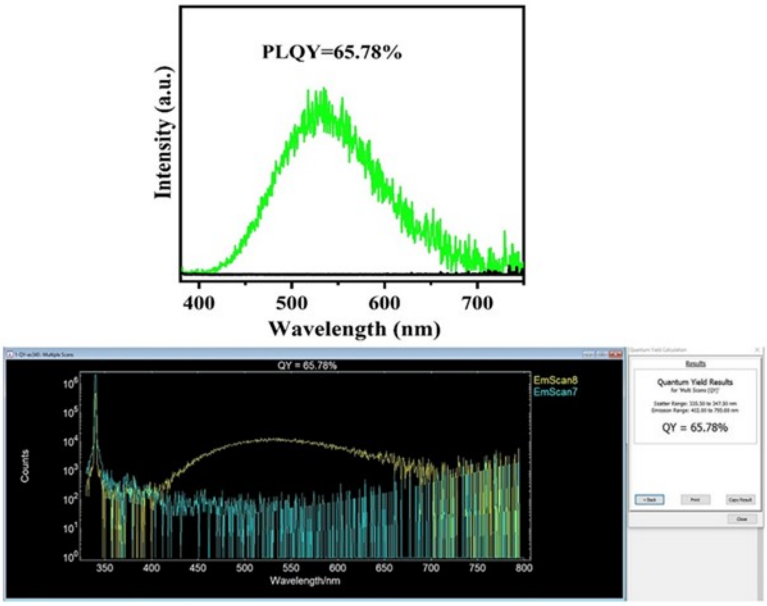

Fig. S5 PLQY of 3% Sb^{3+} single-doped Cs_2KYCl_6 MCs.

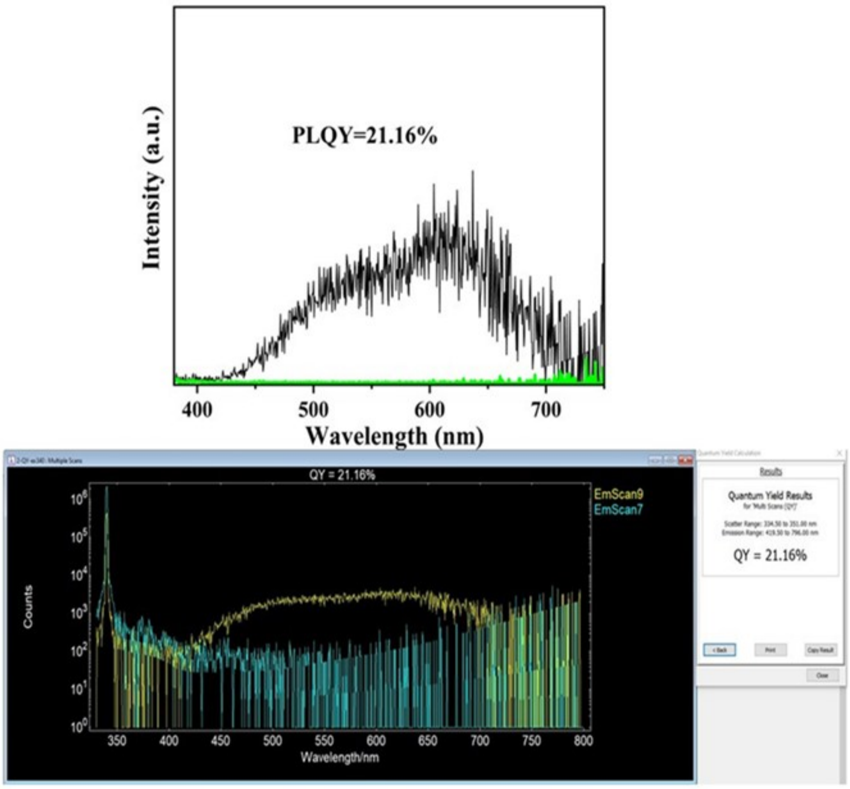

Fig. S6 PLQY spectra of 3% Sb^{3+}/3.5% Mn^{2+} co-doped Cs_2KYCl_6 MCs.

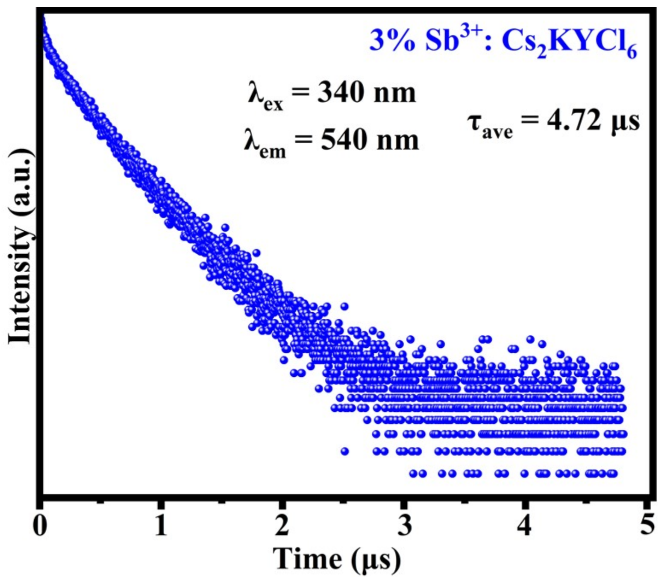

Fig. S7 Time-resolved PL spectra of 3% Sb^{3+} single-doped Cs_2KYCl_6 MCs excited at 340 nm.

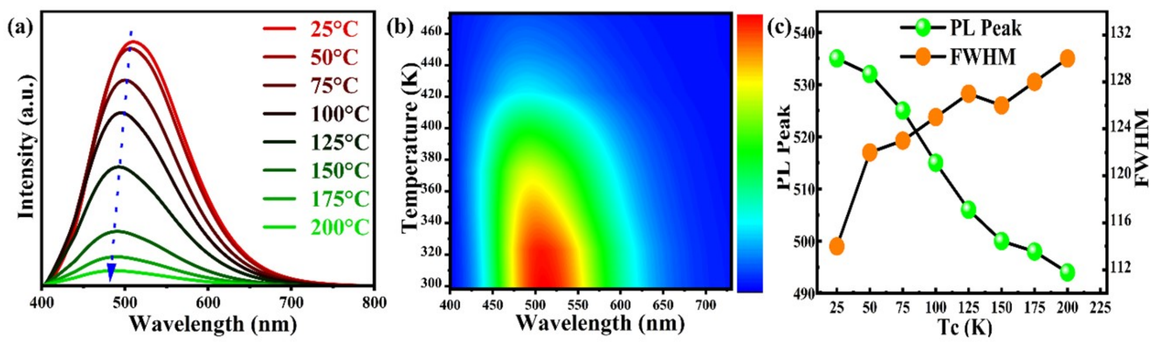

Fig. S8 (a) Temperature-dependent PL of Sb^{3+} single-doped MCs excited at 340 nm. (b) 2D color map of Sb^{3+} single-doped MCs. (c) PL peak positions and FWHM at corresponding temperatures.

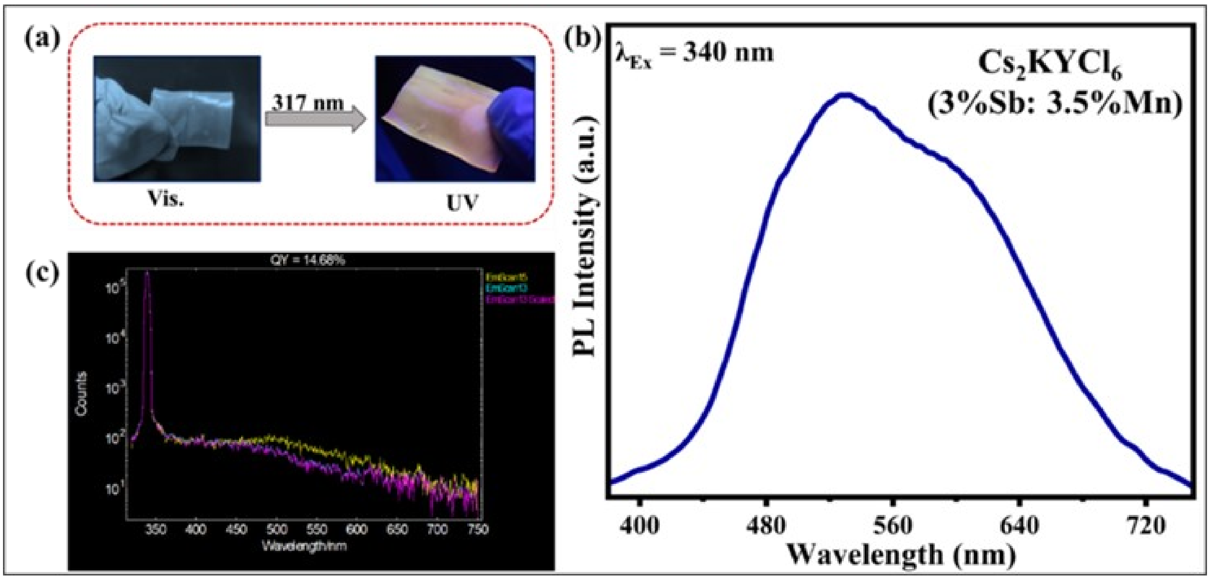

Fig.S9 (a) Thin film of optimal Sb^{3+}/Mn^{2+} co-doped MCs under 317 nm UV radiation (b) PL spectra (c) and PLQY.

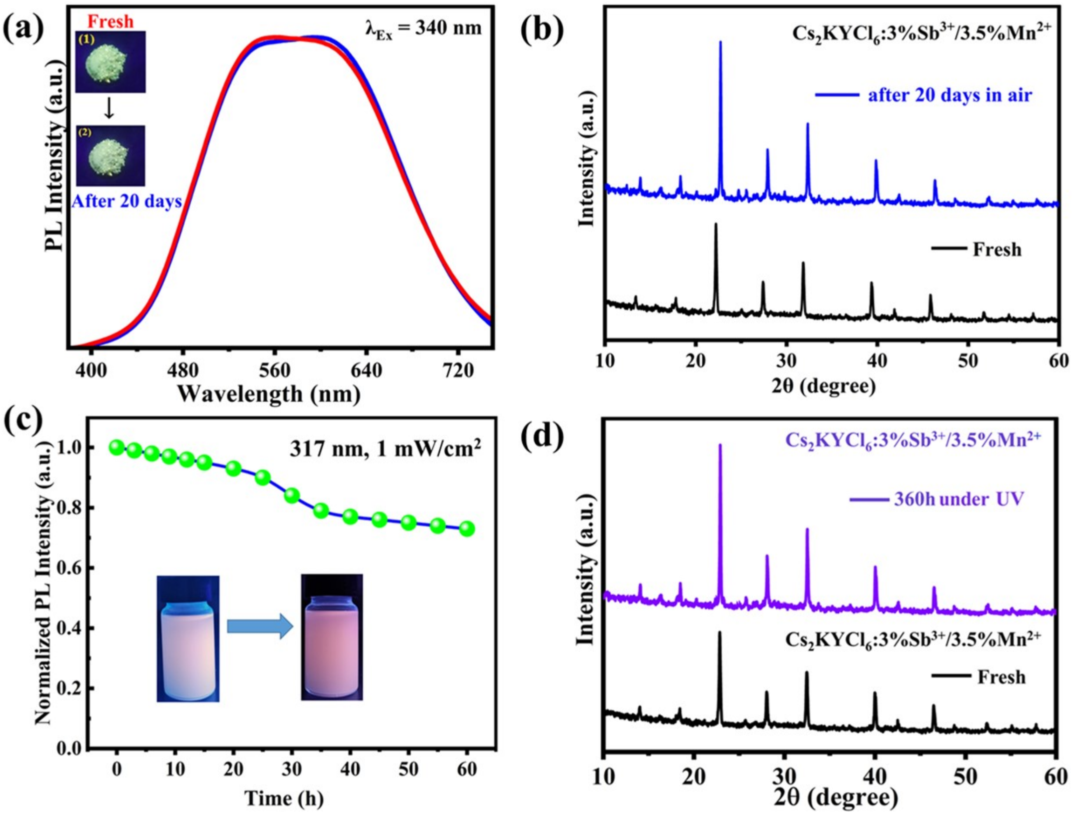

Fig.S10 (a) PL spectra of Sb^{3+}/Mn^{2+} co-doped Cs_2KYCl_6 (fresh and after exposure in the air for 20 days) and (b) XRD after 20 days exposure in the air (c) Normalized PL intensities under continuous light irradiation for 60 h and the insets are photos of pre-and post-test. (d) XRD patterns of the fresh and consecutive 360 h exposure to UV light illumination.

Sites	Formation Energy (eV) Sb^{3+} Defects	Formation Energy (eV) Mn^{2+} Defects
Cs^{3+}	**8.929178 eV**	**-4.9865 eV**
K^{+}	**8.929178 eV**	**5.015505 eV**
Y^{3+}	**- 8.931178 eV**	**-11.6613 eV**
Cl^{-}	**23.87503 eV**	**90.10 eV**
Interstitial	**18.44202 eV**	**68.92 eV**

Table. S1 Formation energies of Sb^{3+} and Mn^{2+} defects in Cs_2KYCl_6

Table. S2 Atomic percentages of 3% Sb^{3+} single-doped Cs_2KYCl_6 MCs

Elements	Cs	K	Y	Cl	Sb
Atomic (%)	21.33	8.52	10.08	59.50	0.56

Table. S3 Atomic percentages of 3% Sb^{3+} and 3.5% Mn^{2+} co-doped Cs_2KYCl_6 MCs.

Elements	Cs	K	Y	Cl	Sb	Mn
Atomic (%)	20.42	4.64	8.06	57.65	2.41	6.82

Table. S4 The average lifetime of 3% Sb^{3+} single-doped Cs_2KYCl_6 MCs at 540 nm excited under 340 nm

t_1 (μs)	t_2 (μs)	A1	A2	τ_{ave} (μs)
0.42	4.91	408.166	760.191	4.72

Table. S5 The average lifetime of 3% Sb^{3+} and 3.5% Mn^{2+} co-doped Cs_2KYCl_6 MCs monitored at 540 nm and 590 nm.

Emission (nm)	t_1 (μs)	t_2 (μs)	A1	A2	τ_{ave} (μs)
540	0.296	4.53	477.13	548.16	4.30
590	0.383	4.929	427.39	382.93	4.57

Components	CIE	CRI	CCT	Ref
Cs_2NaYCl_6: 3%Sb^{3+}/4%Mn^{2+}	(0.34, 0.31)	81.2	5410	[1]
Cs_2SnCl_6:0.59%Sb^{3+}	(0.30, 0.37)	81	6815	[2]
$Cs_2Ag_{0.4}Na_{0.6}InCl_6$:$Bi_3^+$/$Gd^{3+}$	(0.34, 0.33)	93.9	4818	[3]
Cs_2NaYCl_6:1%Sb^{3+}(Eu^{3+}/Tb^{3+})	(0.32, 0.33)	80.3	/	[4]
$Cs_2AgIn_{0.9}Bi_{0.1}Cl_6$	(0.32, 0.32)	94.5	6432	[5]
MA_4In0.9$Sb_{0.1}Cl_7$	(0.39, 0.36)	91	3483	[6]
Cs_2KYCl_6:3%Sb^{3+}/3.5%Mn^{2+}	(0.34, 0.41)	85.4	5062	**This work**

Table. S6. Typical optical features of different lead-free halides WLEDs.

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