Support Information

Excitation-dependent Efficient Photoluminescence in an Organic–Inorganic $(C_4H_{12}N)_2HfCl_6$ Perovskite Induced by Antimony Doping

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Table S1. Crystallographic data and parameters of the Rietveld refinement of $(C_4H_{12}N)_2Hf_{0.95}Cl_6$:$0.05Sb^{3+}$ ($(TMA)_2Hf_{0.95}Cl_6$:$0.05Sb^{3+}$).

Formula	$(C_4H_{12}N)_2Hf_{0.95}Cl_6$:$0.05Sb^{3+}$
crystal system	Cubic
Temperature (K)	298
Space group	*F d -3 c*
a/ Å	25.728844
b/ Å	25.728844
c/ Å	25.728844
α	90.000
β	90.000
γ	90.000
Volume/ $Å^3$	17031.72
2θ-interval,º	5-70
R_p	7.72%
R_{wp}	9.05%
χ^2	1.58

Table S2. Structure parameters for $(TMA)_2Hf_{0.95}Cl_6$:0.05Sb^{3+}.

Structure parameters								
			x	*y*	*z*	Occ.	U	Site
1	Hf	Hf1	0.00000	0.50000	0.00000	0.950	0.065	32c
2	Cl	Cl1	0.00902	0.49101	-0.09415	1.000	0.065	192h
3	N	N1	-0.12500	0.62500	0.12500	1.000	0.052	48d
4	N	N2	-0.12500	0.37500	-0.12500	1.000	0.170	16a
5	C	C1	-0.09190	0.60740	0.16840	1.000	0.063	192h
6	H	H1	-0.07043	0.63554	0.17987	1.000	0.137	192h
7	H	H2	-0.11347	0.59589	0.19655	1.000	0.137	192h
8	H	H3	-0.07041	0.57917	0.15693	1.000	0.137	192h
9	C	C2	-0.15620	0.40620	-0.09380	1.000	0.061	64e
10	H	H4	-0.17773	0.38454	-0.07243	1.000	0.318	192h
11	Sb	Sb1	0.00000	0.50000	0.00000	0.050	0.065	32c

Table S3. PL decay curves for $(TMA)_2Hf_{0.95}Cl_6$:0.05Sb^{3+} monitored at different emission wavelengths.

Sample	Excitation (nm)	Emission Peak (nm)	PL Lifetime (ns)
x = 0.05	320	420	17.44
x = 0.05	320	430	17.60
x = 0.05	320	440	17.66
x = 0.05	320	450	17.78
x = 0.05	320	460	17.87
x = 0.05	320	470	18.01
x = 0.05	320	480	18.07
x = 0.05	320	490	18.23
x = 0.05	320	500	18.36
x = 0.05	320	510	18.49
x = 0.05	320	520	18.63

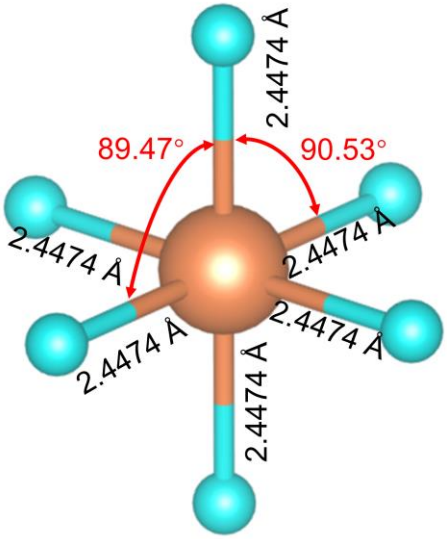

Fig. S1. Multiple specific lengths and included angles of Hf-Cl bond in the $[HfCl_6]^{2-}$ octahedral structure.

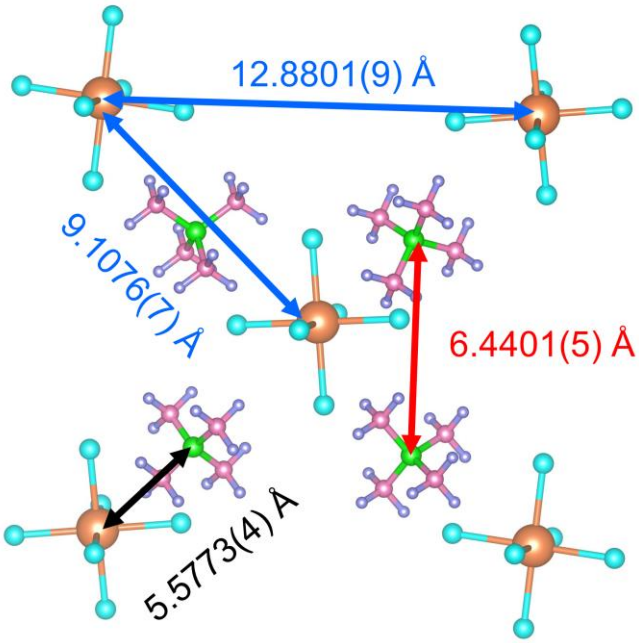

Fig. S2. Crystal structure features of $(TMA)_2HfCl_6$.

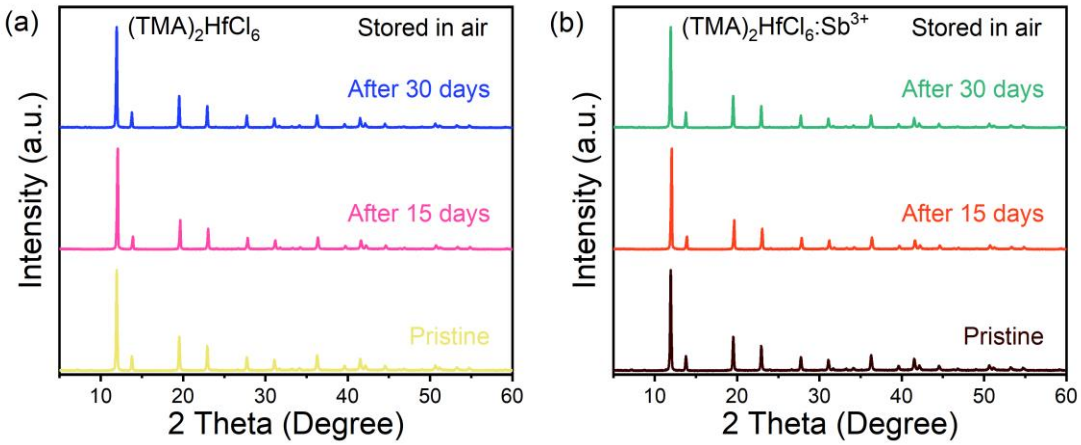

Fig. S3. XRD patterns of (a) $(TMA)_2HfCl_6$ and (b) $(TMA)_2HfCl_6:Sb^{3+}$ after 15 days and 30 days of exposure to light and moisture conditions.

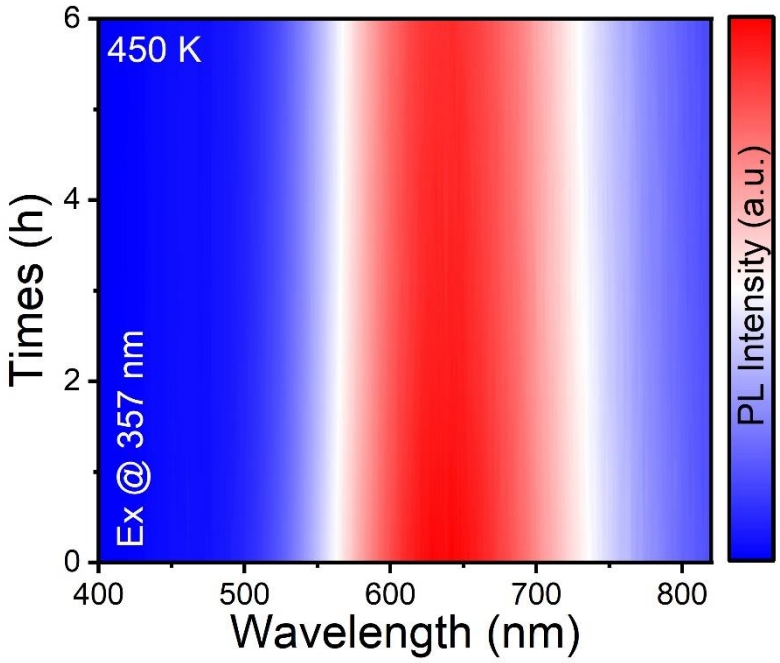

Fig. S4. The PL-temperature correlation map of $(TMA)_2HfCl_6:Sb^{3+}$ maintained at 450 K for 6 h.

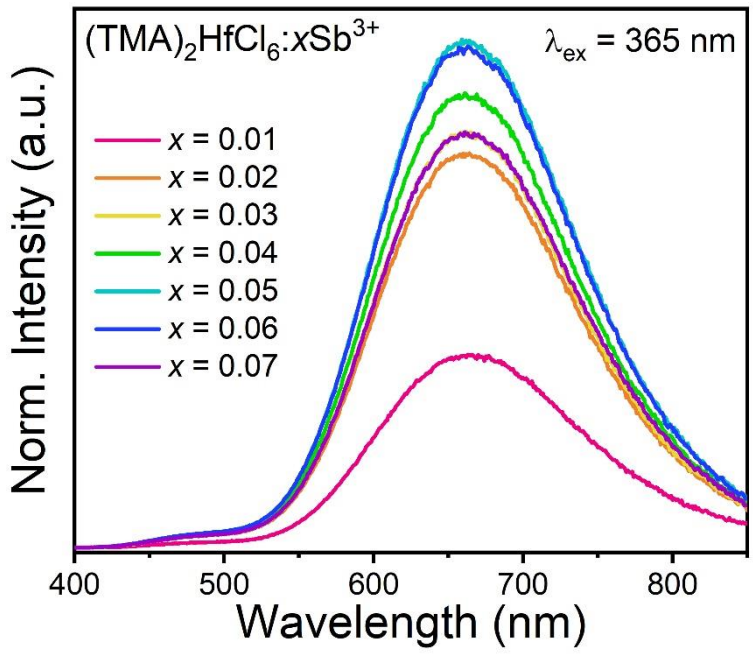

Fig. S5. PL spectra of $(TMA)_2HfCl_6$:$x$$Sb^{3+}$ with different Sb^{3+} concentrations at room temperature (λ_{ex} = 365 nm).

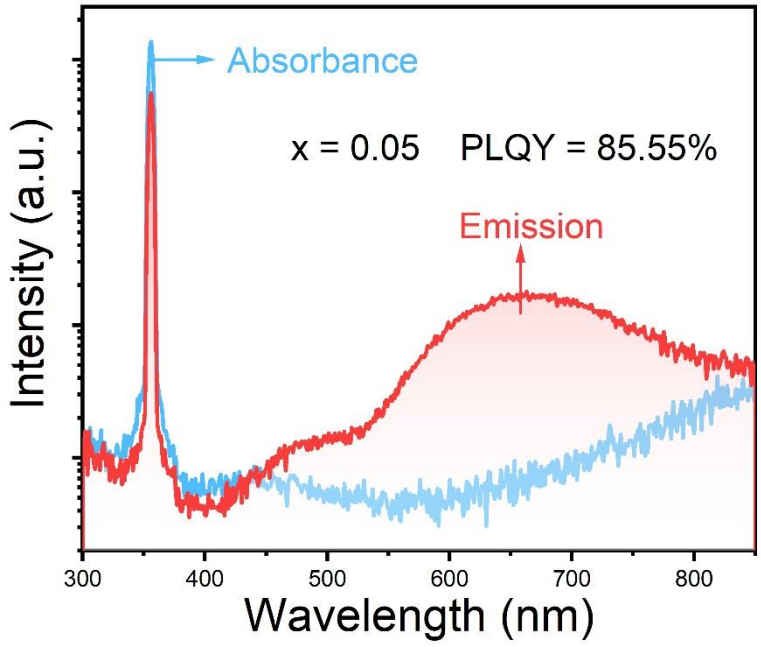

Fig. S6. PL spectra for PLQY of $(TMA)_2HfCl_6$:0.05Sb^{3+} at room temperature.

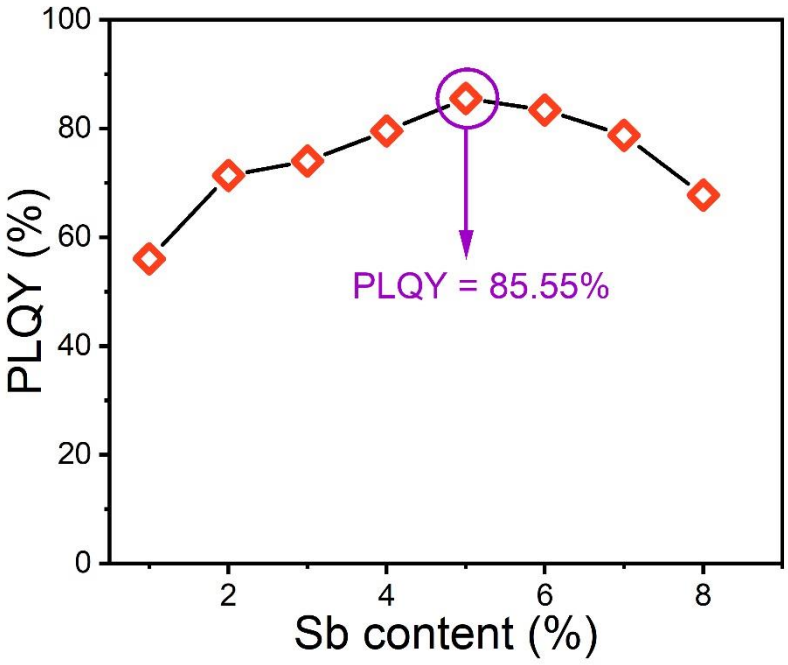

Fig. S7. The PLQY variation of $(TMA)_2HfCl_6$:$x$$Sb^{3+}$ with different Sb^{3+} concentrations upon excitation at 357 nm.

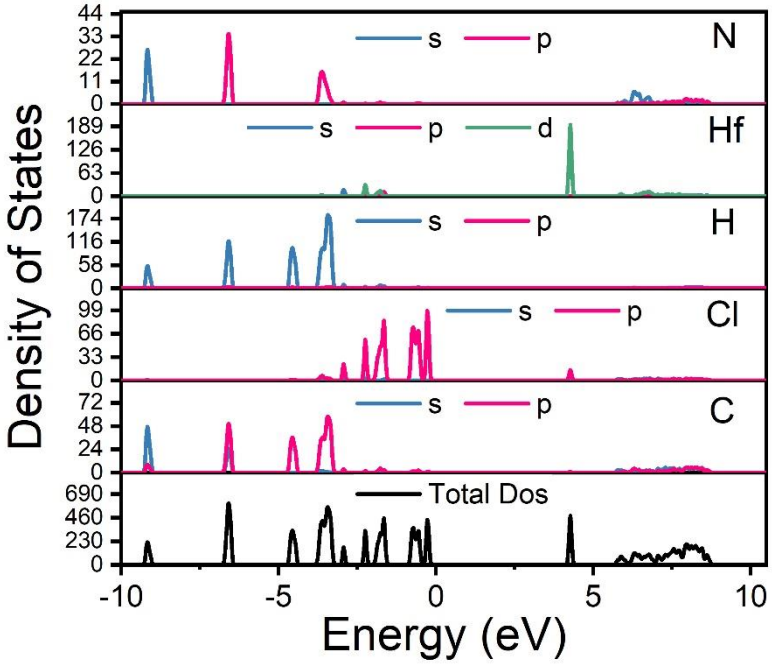

Fig. S8. The total and partial density of states of $(TMA)_2HfCl_6$.

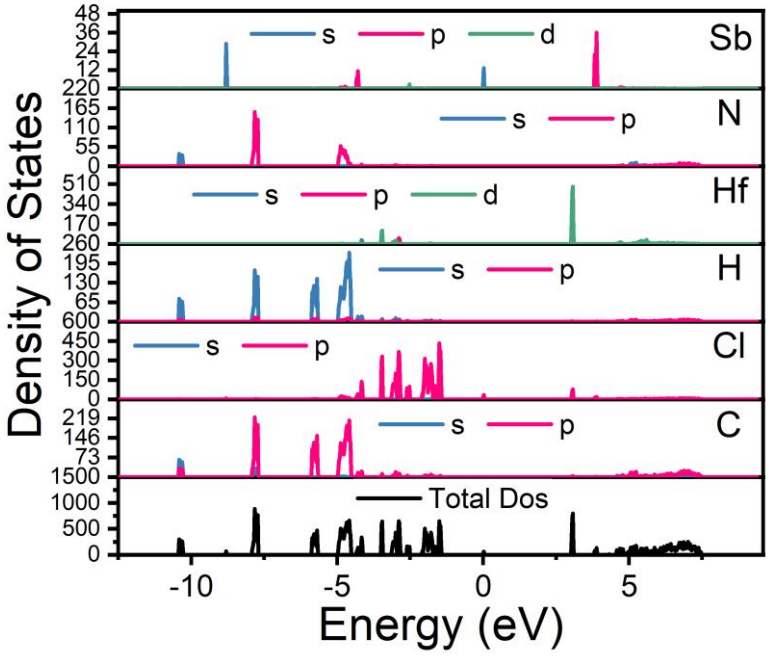

Fig. S9. The total and partial density of states of $(TMA)_2HfCl_6:Sb^{3+}$.