

Competition mechanism of self-trapped excitons and Te^{4+} ions emission in Te^{4+} doped vacancy-ordered double perovskite Rb_2HfCl_6 and its excellent property

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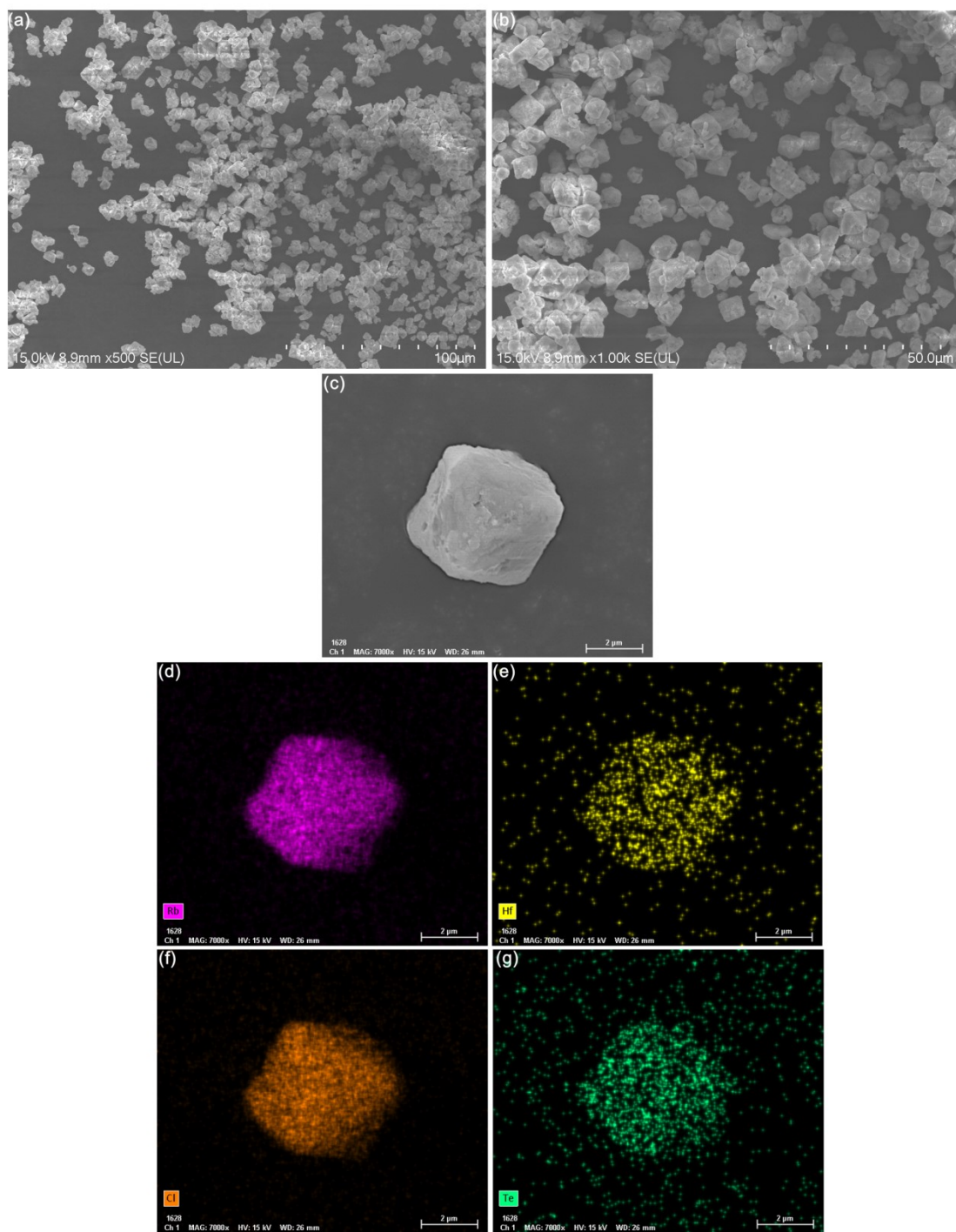


Figure S1. (a,b) SEM images of Rb_2HfCl_6 : 3% Te^{4+} VODP; (c-g) EDS element mapping image for Rb_2HfCl_6 : 3% Te^{4+} .

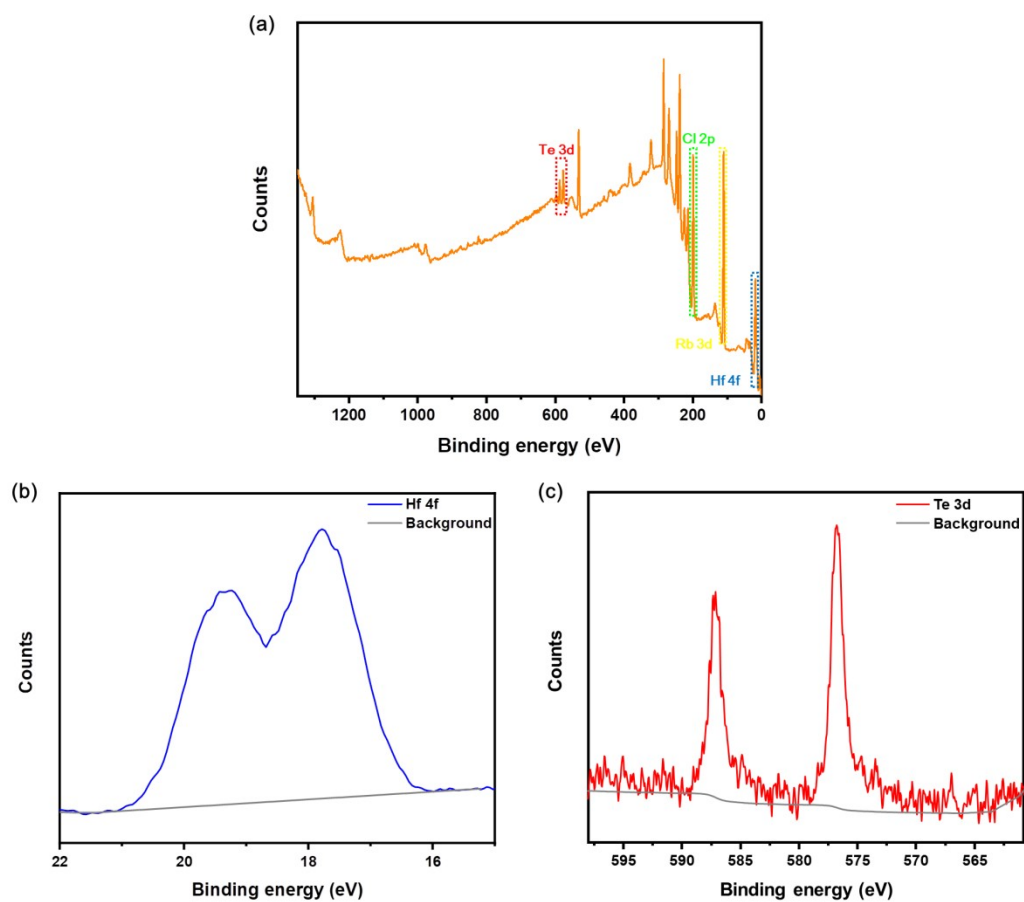


Figure S2. (a) XPS spectrum of $\text{Rb}_2\text{HfCl}_6: 3\%\text{Te}^{4+}\text{VODP}$; High resolution XPS spectrum of (b) $\text{Hf } 4f$ and (c) $\text{Te } 3d$.

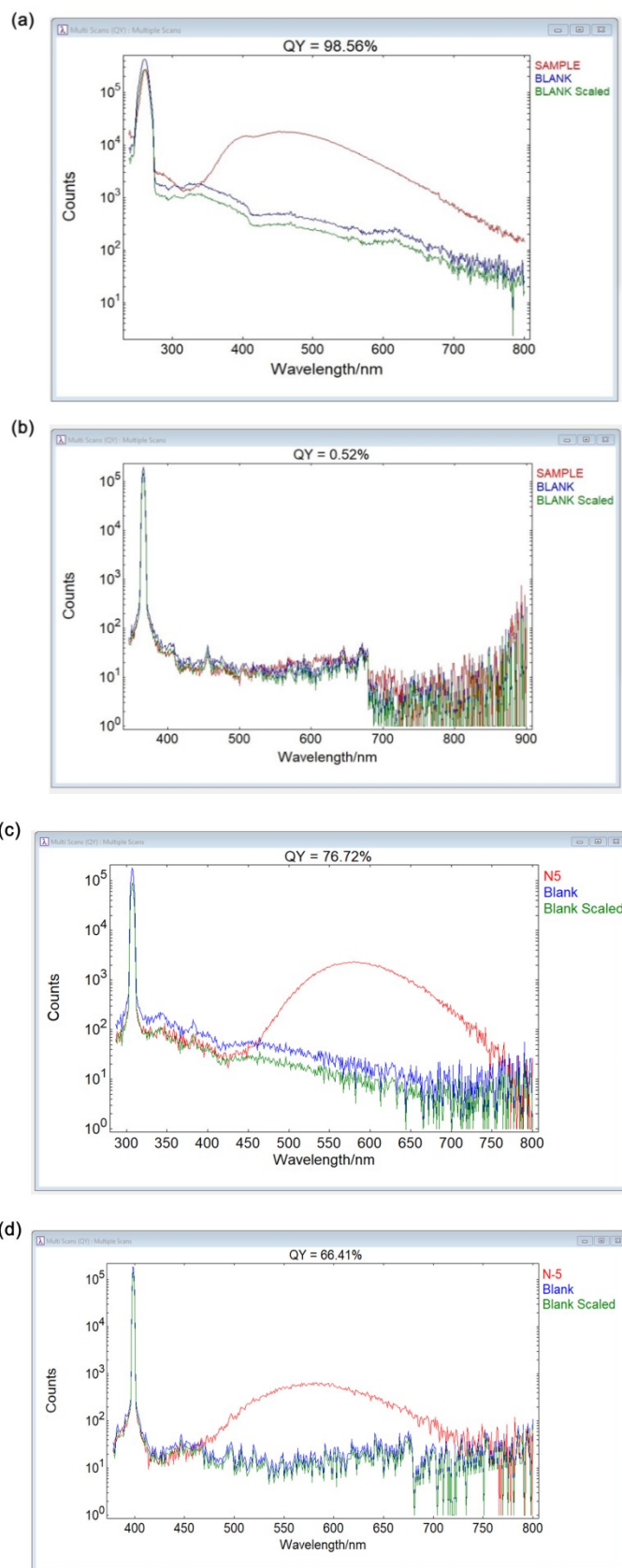


Figure S3. PLQY measurements of (a) Rb_2HfCl_6 and (b) Rb_2TeCl_6 ; PLQY measurement of Rb_2HfCl_6 : 3% Te^{4+} at excitation wavelengths of (c) $\lambda_{\text{ex}} = 306$ nm and (d) $\lambda_{\text{ex}} = 398$ nm.

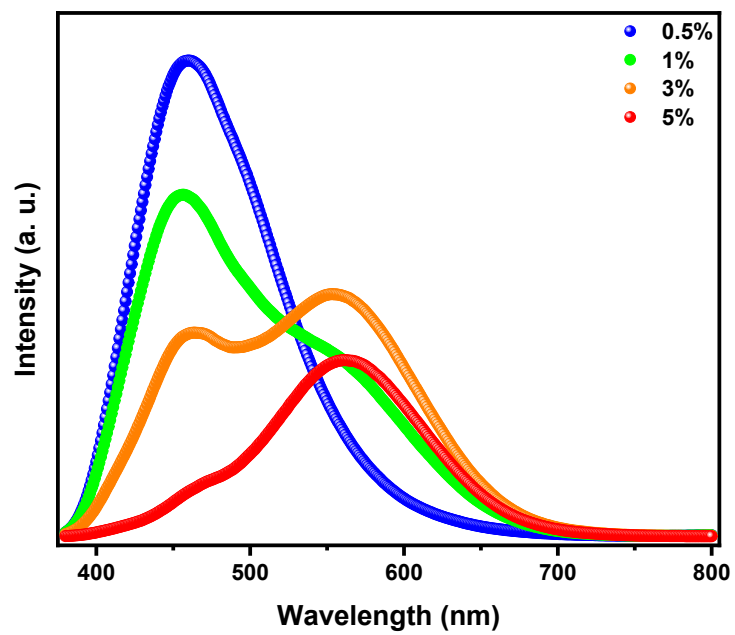


Figure S4. PL spectra of Rb_2HfCl_6 : $x\%\text{Te}^{4+}$ excited by 251 nm ($x=0.5, 1, 3$, and 5).

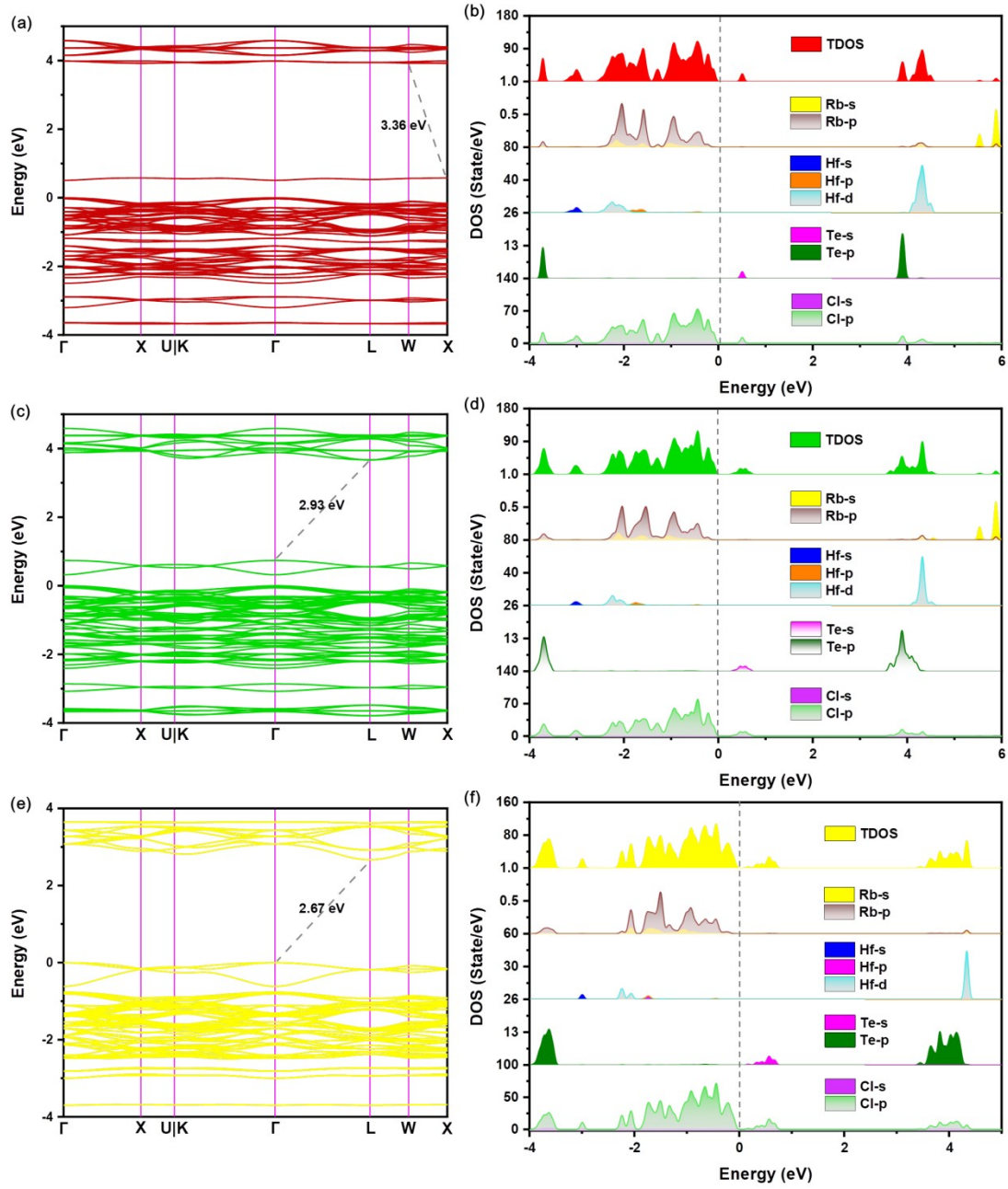


Figure S5. (a) Electronic band structure and (b) DOS of Rb_2HfCl_6 : 25% Te^{4+} ; (c) Electronic band structure and (d) DOS of Rb_2HfCl_6 : 50% Te^{4+} ; (e) Electronic band structure and (f) DOS of Rb_2HfCl_6 : 75% Te^{4+} .

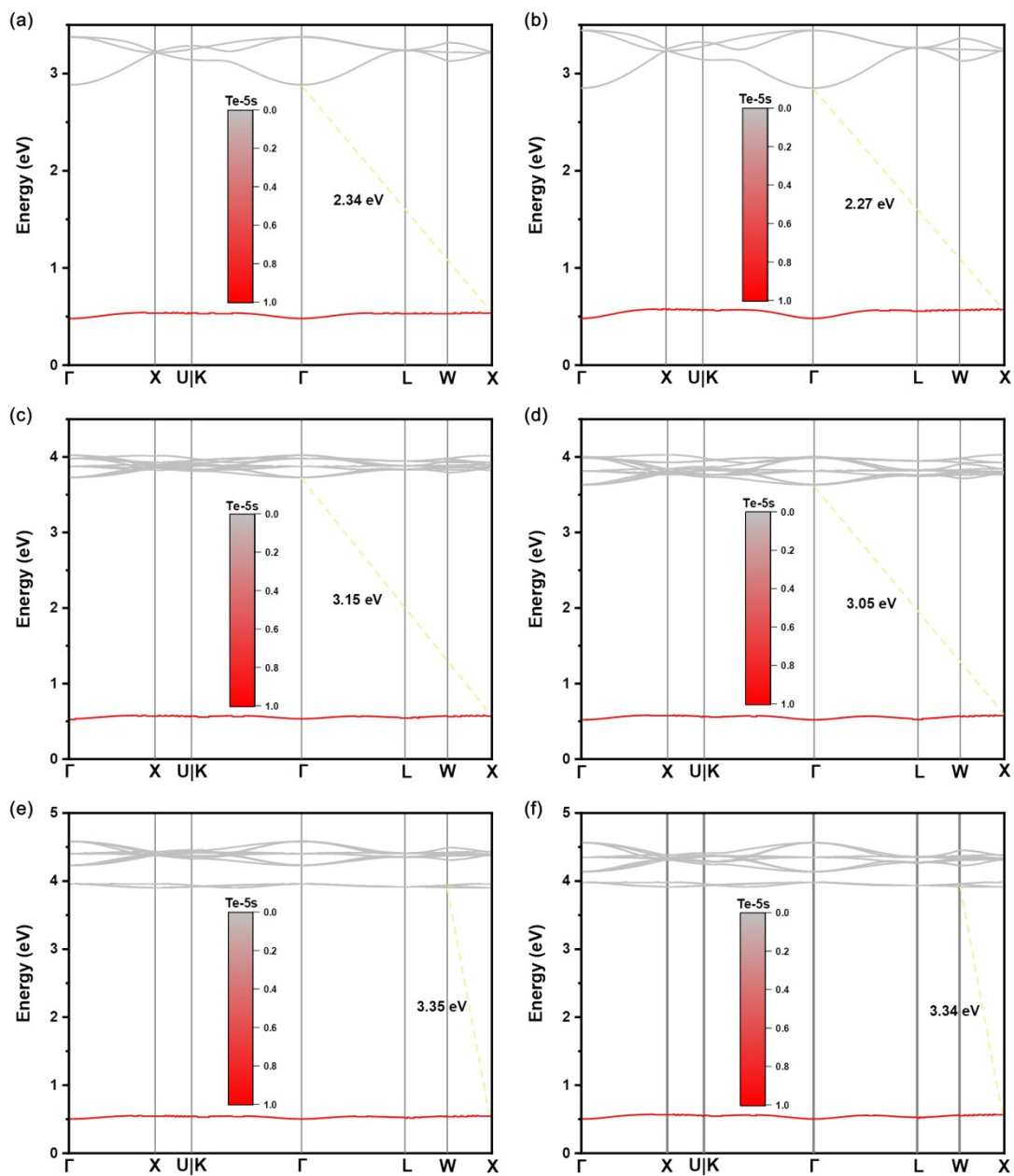


Figure S6. Te-5s orbital projection energy bands of Te-doped (a) Cs_2SnCl_6 , (b) Rb_2SnCl_6 , (c) Cs_2ZrCl_6 , (d) Rb_2ZrCl_6 , (e) Cs_2HfCl_6 and (f) Rb_2HfCl_6 .

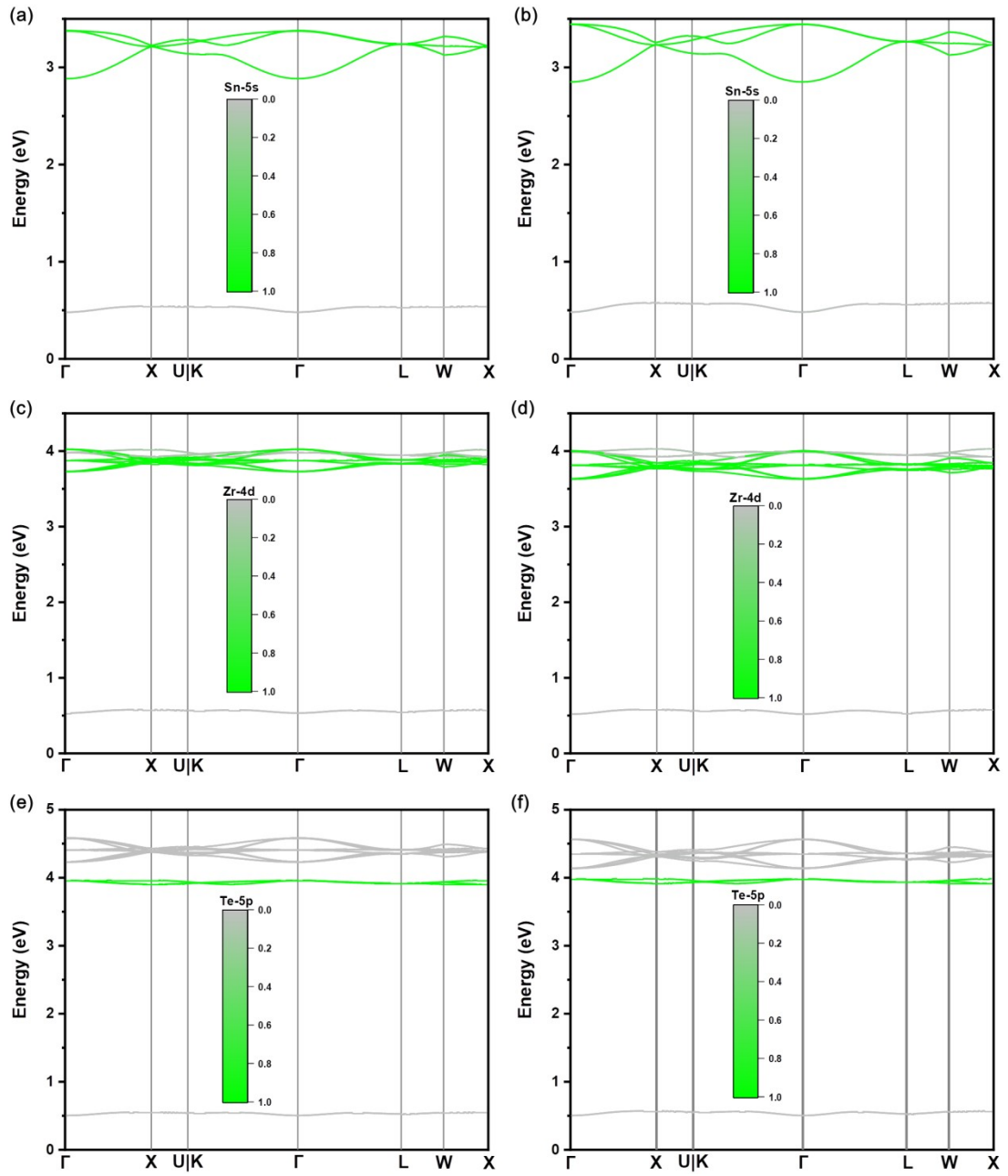


Figure S7. Sn-5s orbital projection energy bands of Te-doped (a) Cs_2SnCl_6 and (b) Rb_2SnCl_6 ; Zr-4d orbital projection energy bands of Te-doped (c) Cs_2ZrCl_6 and (d) Rb_2ZrCl_6 ; Te-5p orbital projection energy bands of Te-doped (e) Cs_2HfCl_6 and (f) Rb_2HfCl_6 .

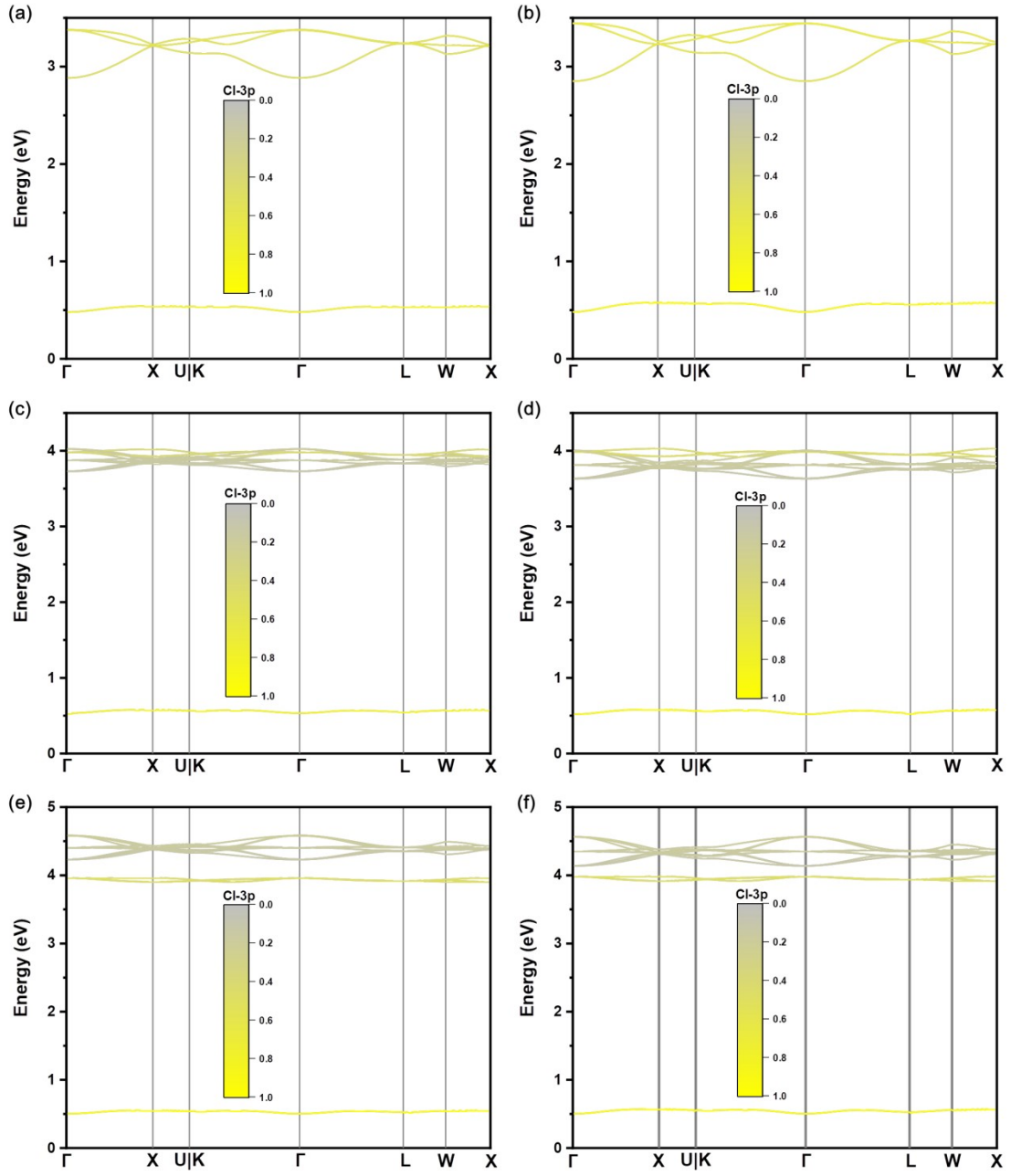


Figure S8. Cl-3p orbital projection energy bands of Te-doped (a) Cs_2SnCl_6 , (b) Rb_2SnCl_6 , (c) Cs_2ZrCl_6 , (d) Rb_2ZrCl_6 , (e) Cs_2HfCl_6 and (f) Rb_2HfCl_6 .

Table S1. The feed ratio of Rb_2HfCl_6 : $x\%\text{Te}^{4+}$ and ICP-OES results.

Feed ratio	ICP-OES results
3%	1.27%
10%	6.74%
25%	19.23%
50%	45.08%
75%	71.61%