Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Photogalvanic effect of 2D van der Waals heterostructure M_2XT_2/SiC by first-principles calculations

Meng Guo[ab], Taifei Zhao[ab], Zhen Cui[ab*],

[a]*School of Automation and Information Engineering,*

Xi'an University of Technology, Xi'an, 710048, P.R. China

[b]*Xi'an Key Laboratory of Wireless Optical Communication and Network Research,*

Xi'an University of Technology, Xi'an, 710048, P.R. China

**Corresponding author: Zhen Cui (Email: zcui@xaut.edu.cn)*

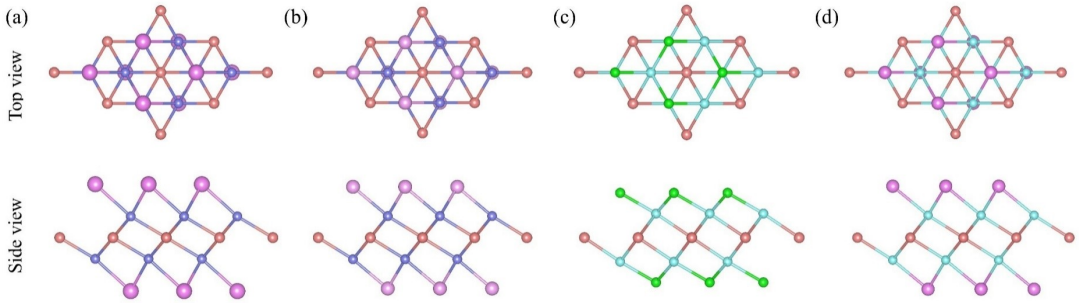

Fig. S1. Optimized top and side views of unit cell for four M_2XT_2 MXenes monolayers (Sc_2CBr_2, Sc_2CCl_2, Y_2CF_2, and Y_2CCl_2). The atoms are color-coded as follows: Sc (blue), Br (purple), Cl (light purple), Y (light blue), and F (cyan).

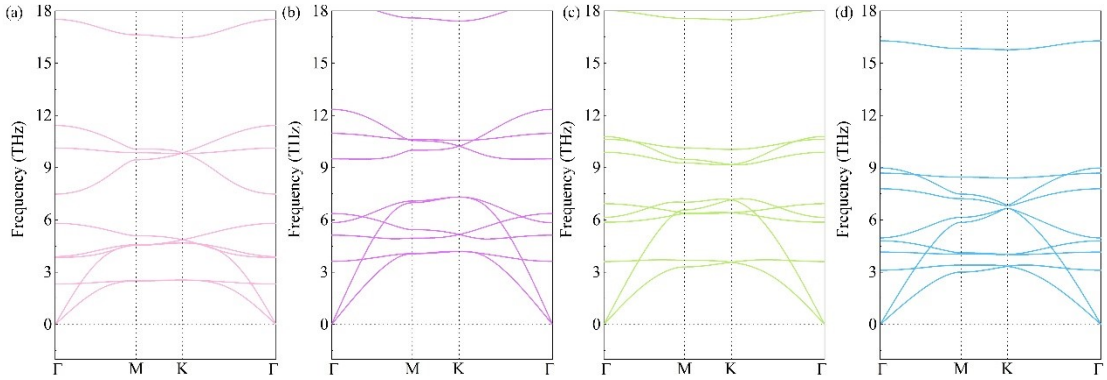

Fig. S2. Phonon dispersion spectra of unit cell for four M_2XT_2 MXenes monolayers (Sc_2CBr_2 (pink lines), Sc_2CCl_2 (purple lines), Y_2CF_2 (cyan lines), and Y_2CCl_2 (blue lines)).

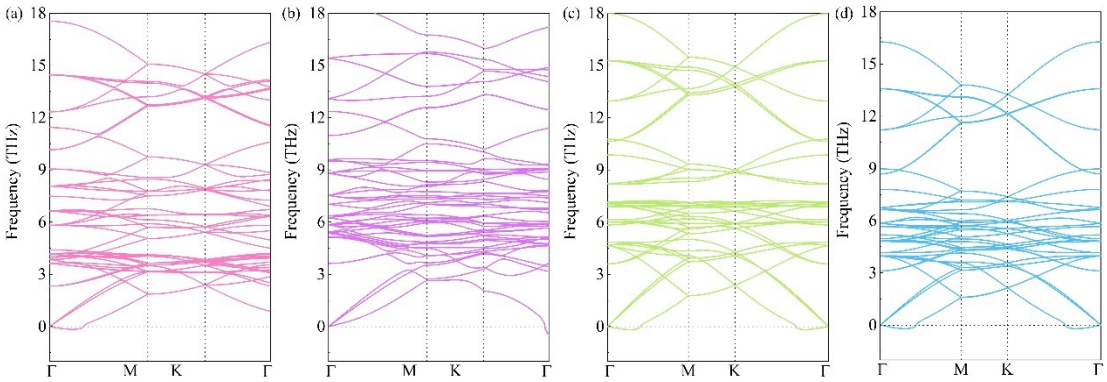

Fig. S3. Phonon dispersion spectra of the supercells for four M_2XT_2 MXenes monolayers (Sc_2CBr_2 (pink lines), Sc_2CCl_2 (purple lines), Y_2CF_2 (cyan lines), and Y_2CCl_2 (blue lines)).

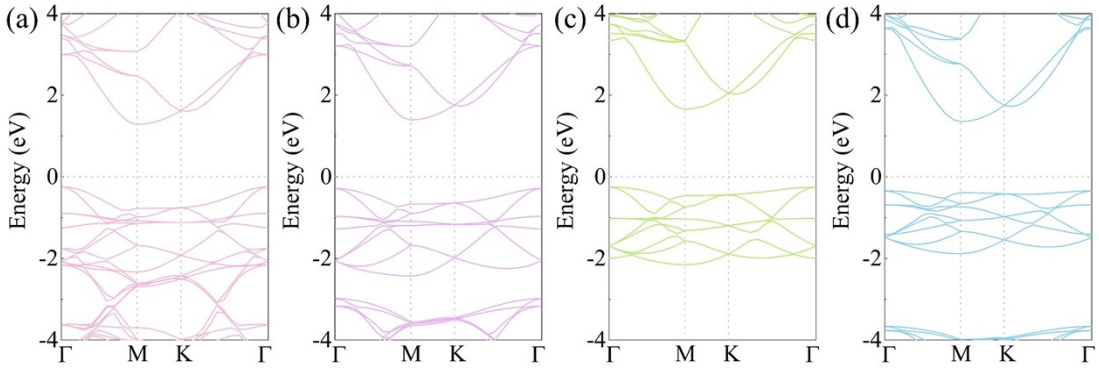

Fig. S4. Band structures of the supercells for four M_2XT_2 MXenes monolayers (Sc_2CBr_2 (pink lines), Sc_2CCl_2 (purple lines), Y_2CF_2 (cyan lines), and Y_2CCl_2 (blue lines)).

Table S1. The structural and electronic parameters including a, PBE bandgaps (E_g^{PBE}), hybrid HSE06 bandgaps (E_g^{HSE}), and VBM/CBM positions of unit cells for isolated monolayers Sc_2CBr_2, Sc_2CCl_2, Y_2CF_2, and Y_2CCl_2.

Type	a (Å)	E_g^{PBE} (eV)	E_g^{HSE} (eV)	VBM/CBM
Sc_2CBr_2	3.52	0.71	1.42	M/ Γ
Sc_2CCl_2	3.43	0.87	1.58	M/ Γ
Y_2CF_2	3.55	1.10	1.81	M/ Γ

Y_2CCl_2	3.69	0.94	1.61	M/ Γ

Table S2. The geometric parameters, including *a*, E_g^{PBE}, E_g^{HSE}, and VBM/CBM positions for supercells Sc_2CBr_2, Sc_2CCl_2, Y_2CF_2, and Y_2CCl_2.

Type	*a* (Å)	E_g^{PBE} (eV)	E_g^{HSE} (eV)	VBM/CBM
Sc_2CBr_2	6.08	0.70	1.52	M/ Γ
Sc_2CCl_2	5.95	0.87	1.68	M/ Γ
Y_2CF_2	6.15	1.11	1.91	M/ Γ
Y_2CCl_2	6.39	0.94	1.69	M/ Γ

Table S3. The formation energies of all configurations of the four types of HJs under different stacking schemes.

Model	Pattern-A	Pattern-B	Pattern-C	Pattern-D	Pattern-E	Pattern-F
Sc_2CBr_2/SiC	-3.298	-3.298	-3.298	-3.300	-3.298	-3.300
Sc_2CCl_2/SiC	-2.657	-2.658	-2.658	-2.659	-2.658	-2.658
SiC/Y_2CF_2	-0.856	-0.857	-0.857	-0.857	-0.859	-0.858
SiC/Y_2CCl_2	-0.624	-0.624	-0.624	-0.624	-0.625	-0.624

Table S4. The *a*, E_g^{PBE} (eV), E_g^{HSE} (eV), and *Φ* of Sc_2CBr_2/SiC, Sc_2CCl_2/SiC, SiC/Y_2CF_2, and SiC/Y_2CCl_2 after optimization.

Type	*a* (Å)	E_g^{PBE} (eV)	E_g^{HSE} (eV)	*Φ (eV)*
Sc_2CBr_2/SiC	6.14	0.19	0.87	4.99
Sc_2CCl_2/SiC	6.07	0.04	0.72	5.09
SiC/Y_2CF_2	6.17	1.14	1.94	4.19
SiC/Y_2CCl_2	6.27	0.11	0.77	5.06

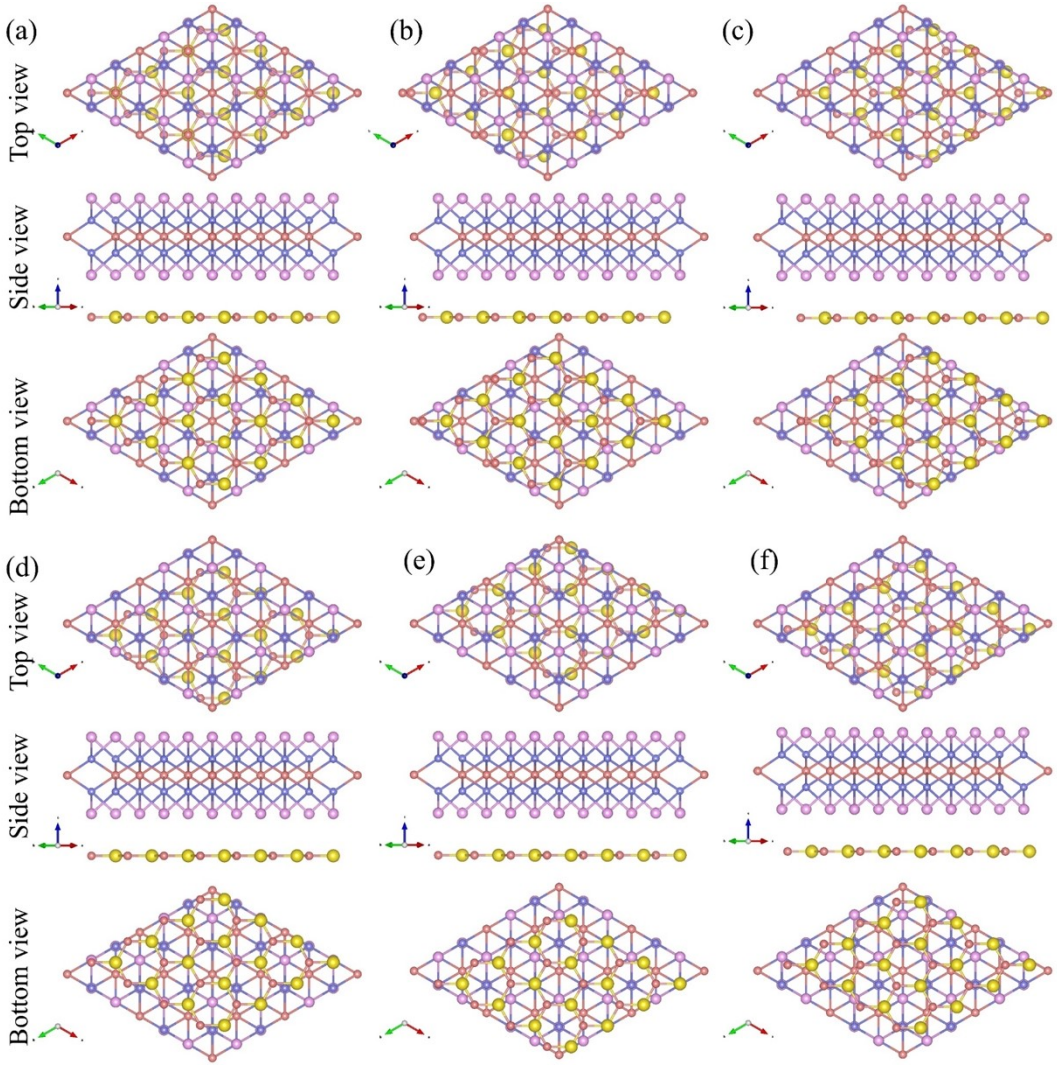

Fig. S5. Six vertical stacking models of Sc_2CCl_2/SiC HJ. The atoms are color-coded as follows: Si (yellow), C (orange), Sc (blue), and Cl (light purple).

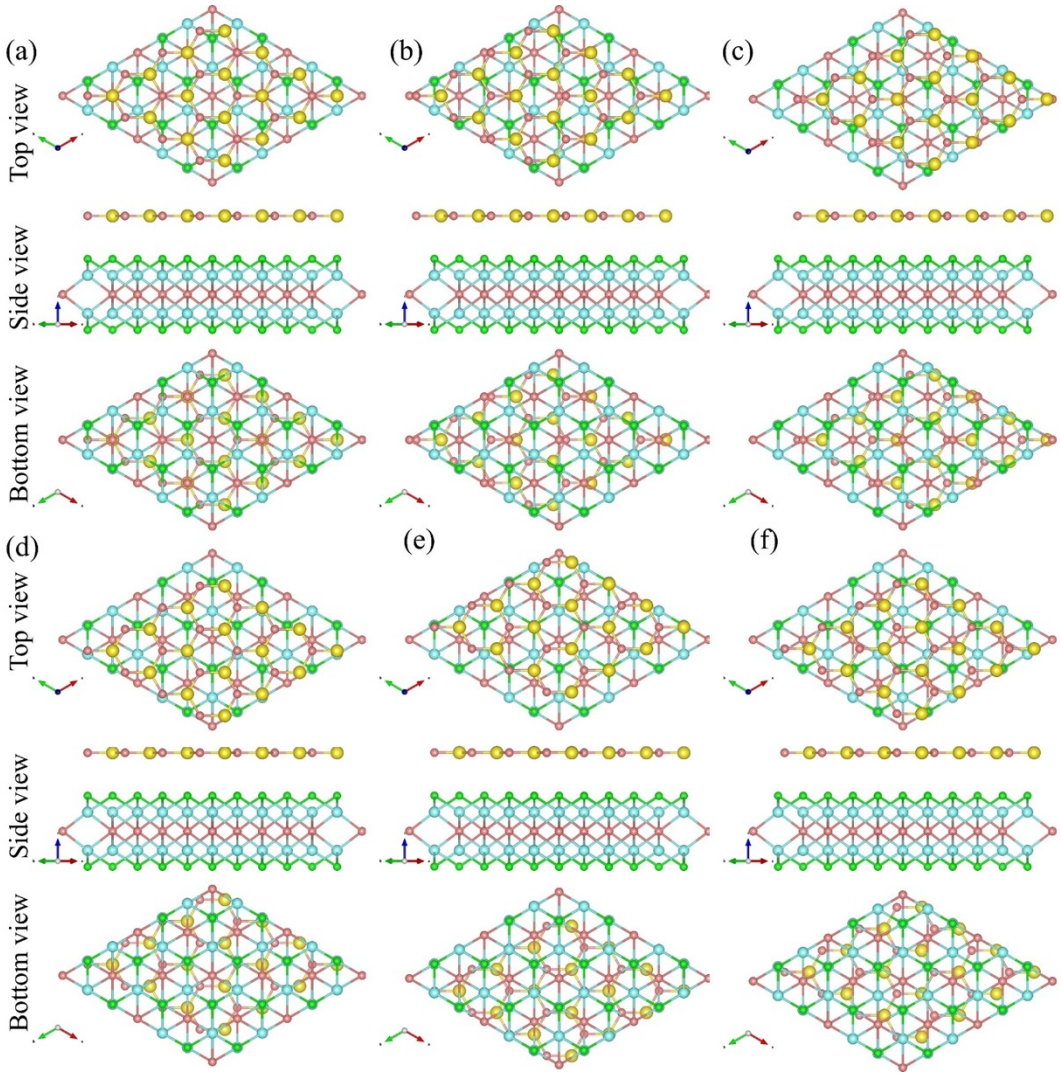

Fig. S6. Six vertical stacking models of SiC/Y_2CF_2 HJ. The atoms are color-coded as follows: Si (yellow), C (orange), Y (light blue), and F (cyan).

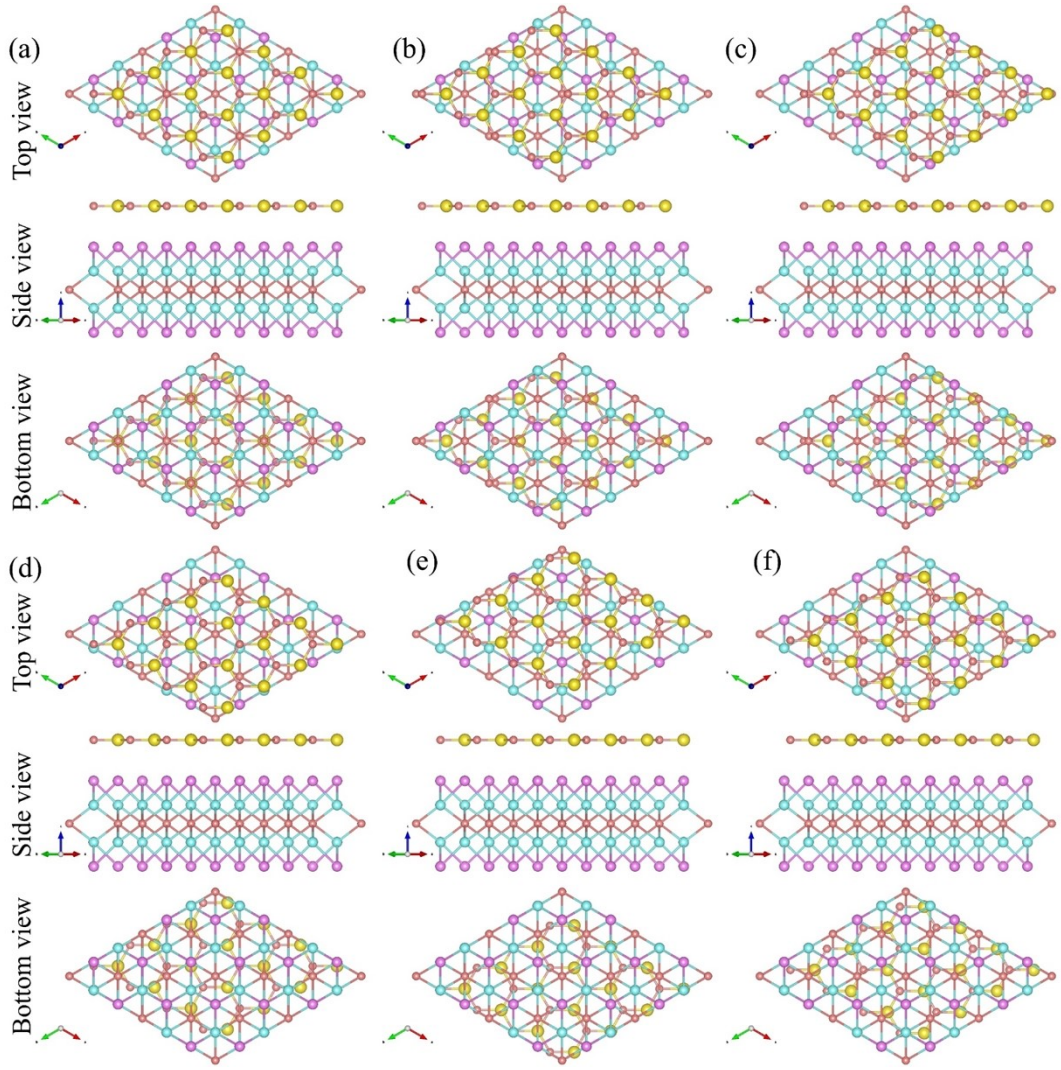

Fig. S7. Six vertical stacking models of SiC/Y_2CCl_2 HJ. The atoms are color-coded as follows: Si (yellow), C (orange), Cl (light purple), and Y (light blue).

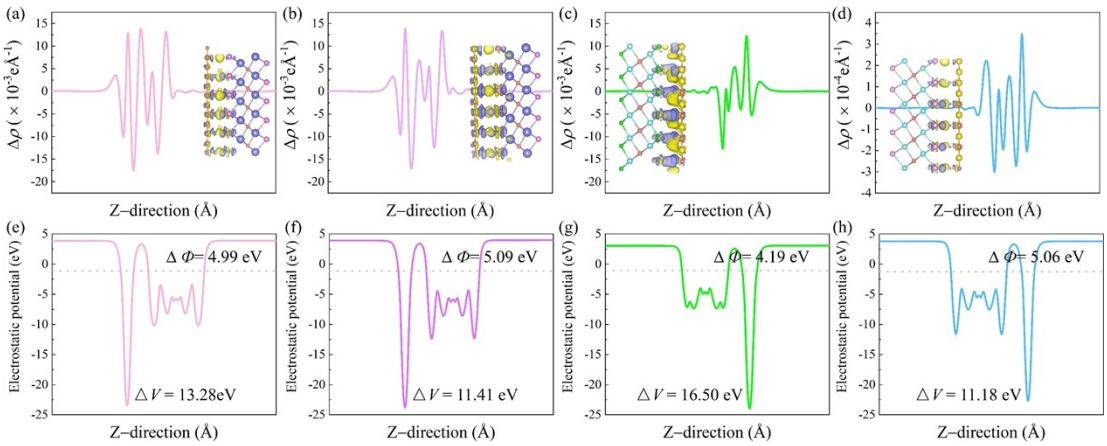

Fig. S8. The Plane-averaged CD and electrostatic potential staggered of Sc_2CBr_2/SiC (pink lines), Sc_2CCl_2/SiC (purple lines), SiC/Y_2CF_2 (cyan lines), and SiC/Y_2CCl_2 (blue lines) after optimization.

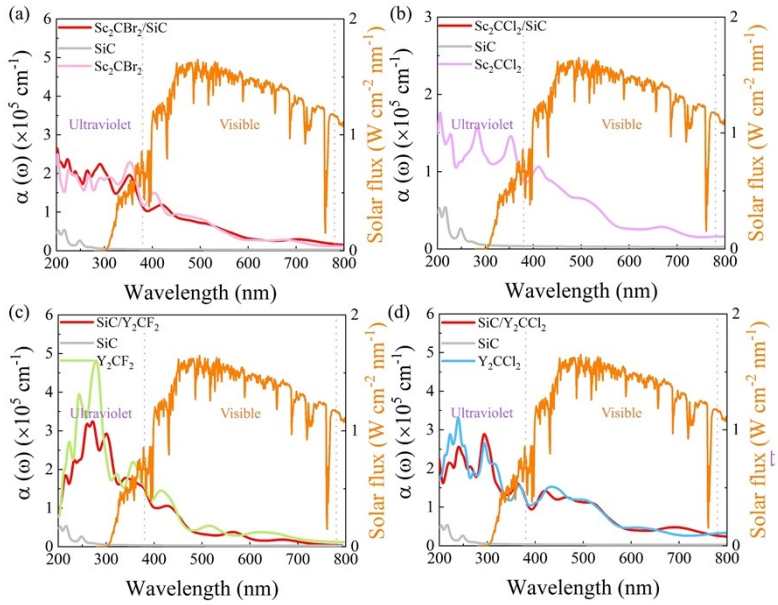

Fig. S9. The optical absorption spectrum of Sc_2CBr_2, Sc_2CCl_2, Y_2CF_2, Y_2CCl_2, SiC, Sc_2CBr_2/SiC, Sc_2CCl_2/SiC, SiC/Y_2CF_2, and SiC/Y_2CCl_2 after optimization.

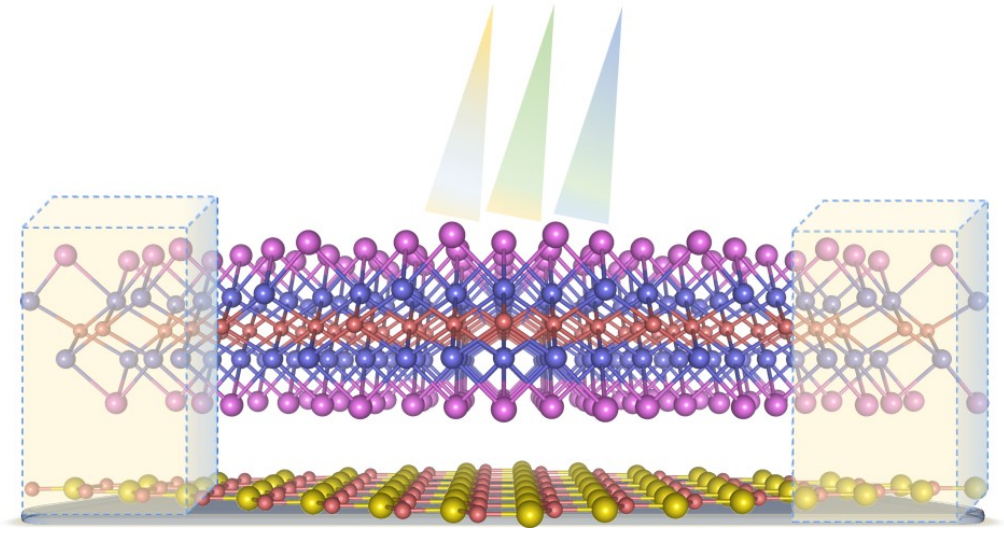

Fig. S10. Photocurrent model of Sc_2CBr_2/SiC, Sc_2CCl_2/SiC, SiC/Y_2CF_2, and SiC/Y_2CCl_2 HJs.