

*Electronic Supplementary Material for*

# **First-principles study on Janus structured $\text{Sc}_2\text{CX}_2/\text{Sc}_2\text{CY}_2$ (X, Y = F, Cl, Br) Heterostructures for Solar Energy Conversion**

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Table S1. The structure coordinate information (POSCAR) of the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CCL}_2$  heterostructure with three different stacking configurations. The POSCAR of  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CBr}_2$  and  $\text{Sc}_2\text{CCL}_2/\text{Sc}_2\text{CBr}_2$  heterostructures are the same as those of the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CCL}_2$  heterostructure.

A			
1.0			
3.2667000294	0.0000000000	0.0000000000	
-1.6333500147	2.8290452120	0.0000000000	
0.0000000000	0.0000000000	39.9822006226	
Sc	F	Cl	C
4	2	2	2
Direct			
0.333333343	0.666666687	0.637989998	
0.333333343	0.666666687	0.442160010	
0.666666687	0.333333343	0.574590027	
0.666666687	0.333333343	0.378760010	
0.333333343	0.666666687	0.545889974	
0.666666687	0.333333343	0.666666687	
0.333333343	0.666666687	0.350059986	
0.666666687	0.333333343	0.470860004	
0.000000000	0.000000000	0.606289983	
0.000000000	0.000000000	0.410459995	

B			
1.0			
3.2667000294	0.0000000000	0.0000000000	
-1.6333500147	2.8290452120	0.0000000000	
0.0000000000	0.0000000000	39.9822006226	
Sc	F	Cl	C
4	2	2	2
Direct			
0.666666687	0.333333343	0.637989998	
0.666666687	0.333333343	0.378760010	
0.333333343	0.666666687	0.442160010	
0.000000000	0.000000000	0.574590027	
0.666666687	0.333333343	0.545889974	
0.000000000	0.000000000	0.666666687	
0.666666687	0.333333343	0.470860004	
0.333333343	0.666666687	0.350059986	
0.333333343	0.666666687	0.606289983	
0.000000000	0.000000000	0.410459995	

C			
1.0			
3.2667000294	0.0000000000	0.0000000000	
-1.6333500147	2.8290452120	0.0000000000	
0.0000000000	0.0000000000	39.9822006226	
Sc	F	Cl	C
4	2	2	2
Direct			
0.000000000	0.000000000	0.637989998	
0.333333343	0.666666687	0.442160010	
0.333333343	0.666666687	0.574590027	
0.666666687	0.333333343	0.378760010	
0.000000000	0.000000000	0.545889974	
0.333333343	0.666666687	0.666666687	
0.333333343	0.666666687	0.350059986	
0.666666687	0.333333343	0.470860004	
0.666666687	0.333333343	0.606289983	
0.000000000	0.000000000	0.410459995	

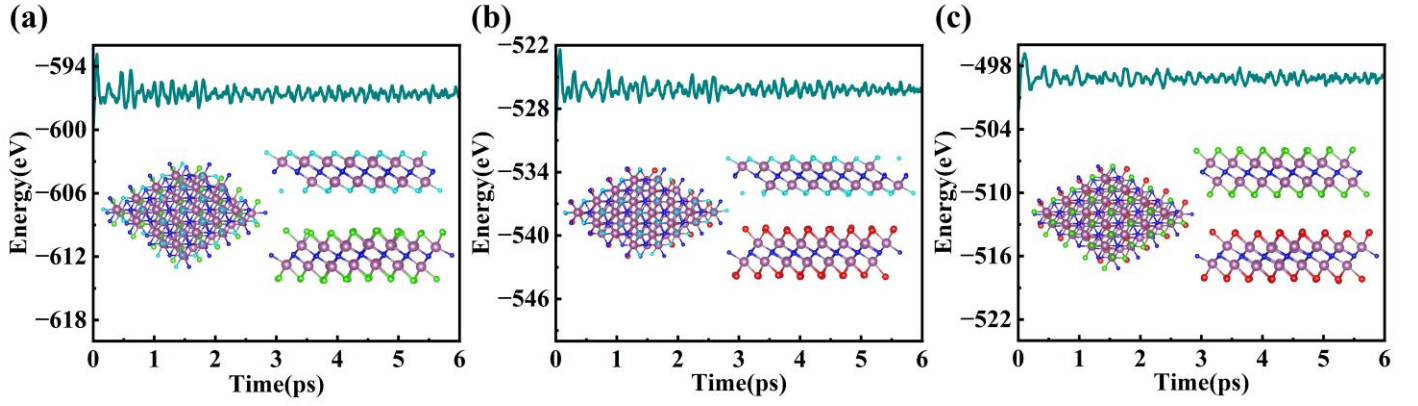


Figure S1. (a-c) AIMD fluctuations of the total energy for the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CCl}_2$ ,  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CBr}_2$ , and  $\text{Sc}_2\text{CCl}_2/\text{Sc}_2\text{CBr}_2$  heterostructures at 300 K with 6ps. The insets are top and side views of the final structures in the AIMD simulation.

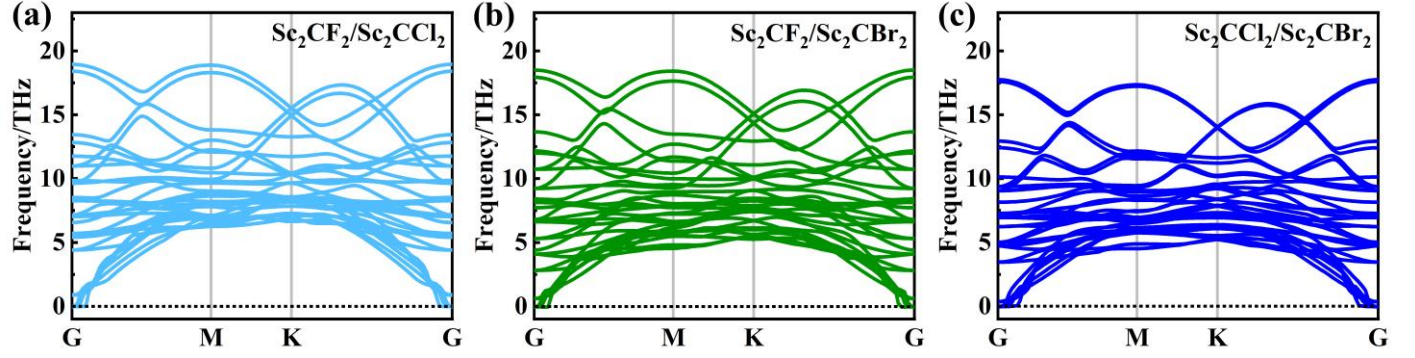


Figure S2. (a-c) Phonon dispersion structures of the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CCl}_2$ ,  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CBr}_2$ , and  $\text{Sc}_2\text{CCl}_2/\text{Sc}_2\text{CBr}_2$  heterostructures.

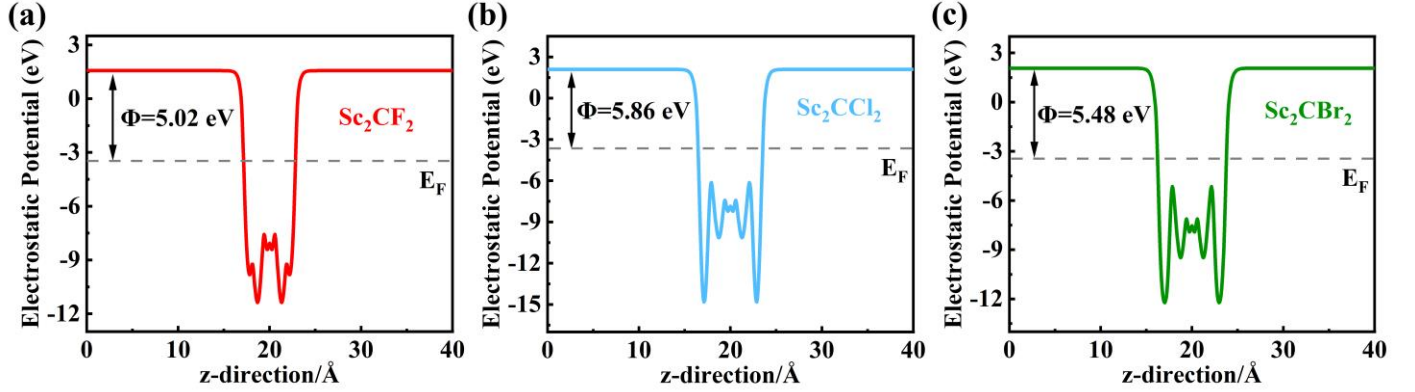


Figure S3. Electrostatic potential for (a)  $\text{Sc}_2\text{CF}_2$ , (b)  $\text{Sc}_2\text{CCl}_2$ , and (c)  $\text{Sc}_2\text{CBr}_2$  monolayers.

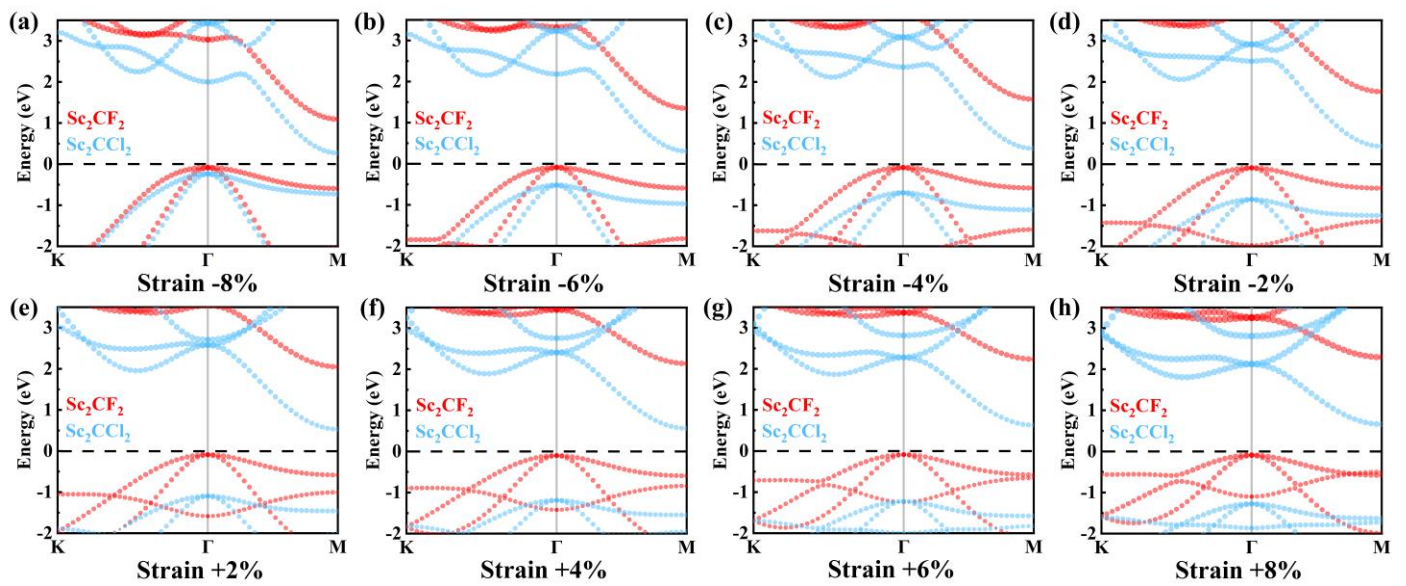


Figure S4. Relation between band gap of the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CCl}_2$  heterostructure and biaxial strain.

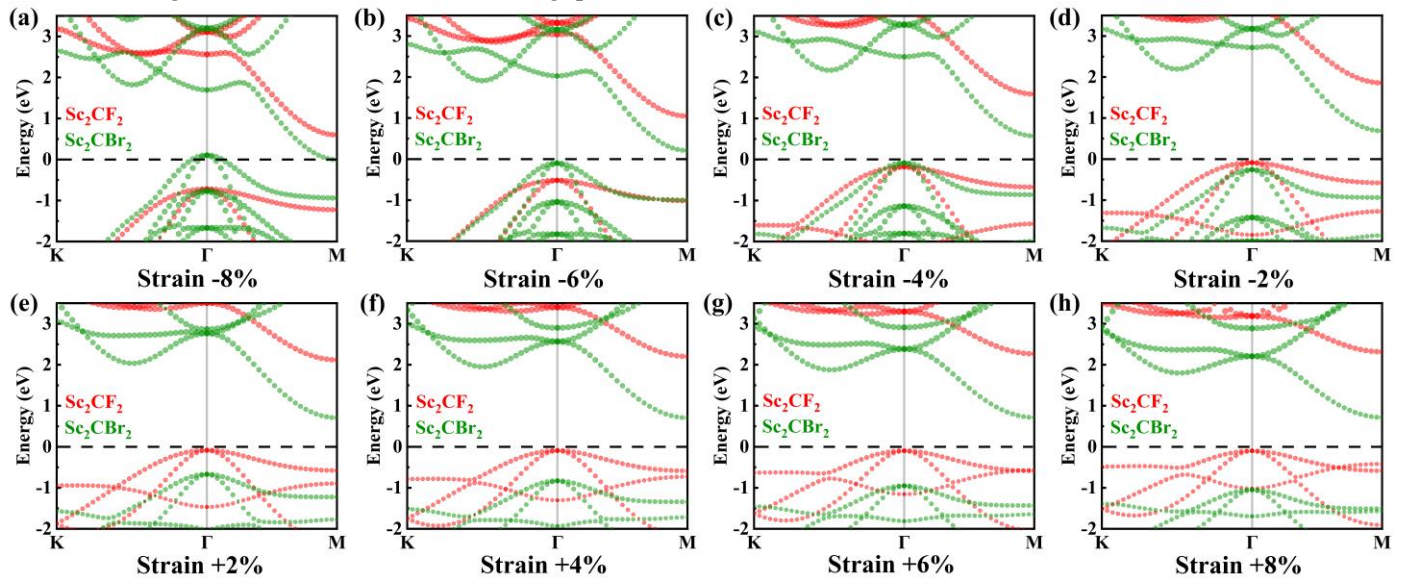


Figure S5. The projected band structures of the  $\text{Sc}_2\text{CF}_2/\text{Sc}_2\text{CBr}_2$  heterostructure under different vertical strains.

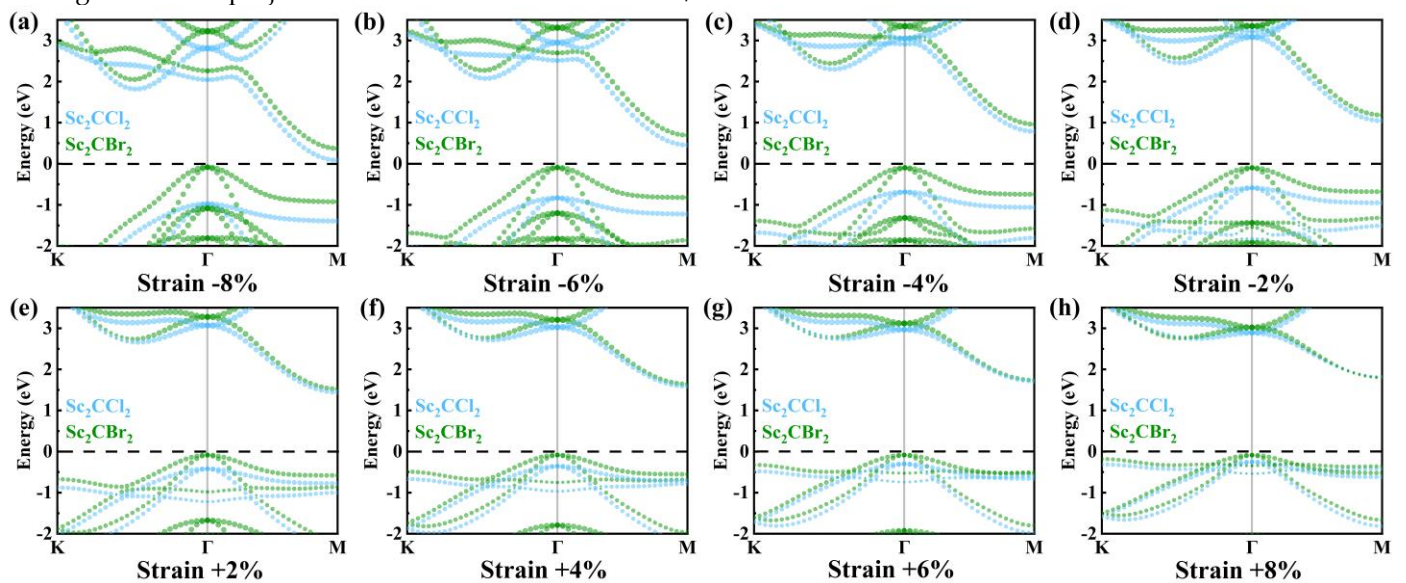


Figure S6. Energy bands of the  $\text{Sc}_2\text{CCl}_2/\text{Sc}_2\text{CBr}_2$  heterostructure under different strains.

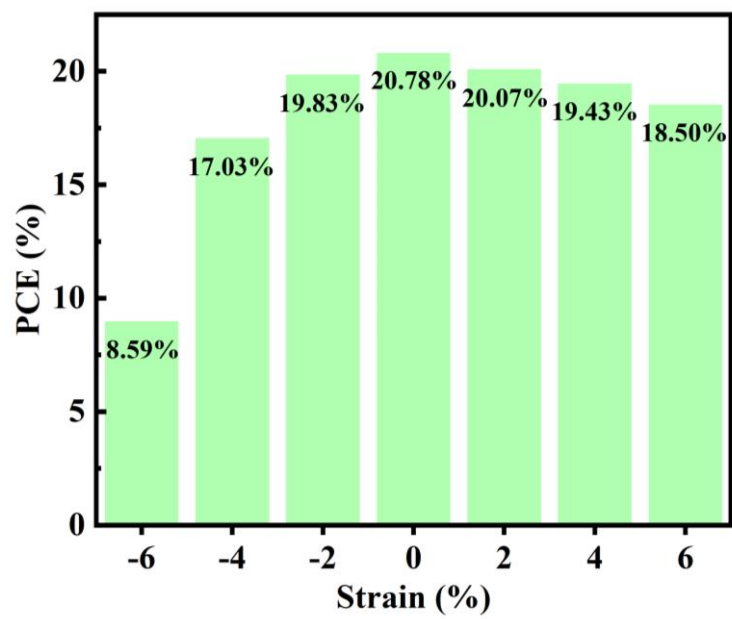


Figure S7. The PCE of the Sc<sub>2</sub>CCl<sub>2</sub>/Sc<sub>2</sub>CBr<sub>2</sub> heterostructure with different strains.