Supplementary Information

Ferroelectric heterointerface control of spin polarization in Janus antiferromagnet and its application in multistate storage†

Huan Xiao,[1, 2] Jialong Qi,[1, 2] Lili Kang,[1, 2, a)] Gaofeng Zhao,[1, 2, 3, b)] and Peng Jiang[4, c)]

1)Key Laboratory for High Efficiency Energy Conversion Science and Technology of Henan Province, School of Physics and Electronics, Henan University, Kaifeng 475004, China

2)International Joint Research Laboratory of New Energy Materials and Devices of Henan Province, School of Physics and Electronics, Henan University, Kaifeng 475004, China

3)School of Flexible Electronics (SoFE) and Henan Institute of Flexible Electronics (HIFE), Henan University, 379 Mingli Road, Zhengzhou 450046, China

4)School of Physics and Electronic Engineering, Jiangsu Normal University, Xuzhou 221116, China

a) Electronic mail: llkang@henu.edu.cn
b) Electronic mail: gfzhao@henu.edu.cn
c) Electronic mail: pjiang@jsnu.edu.cn

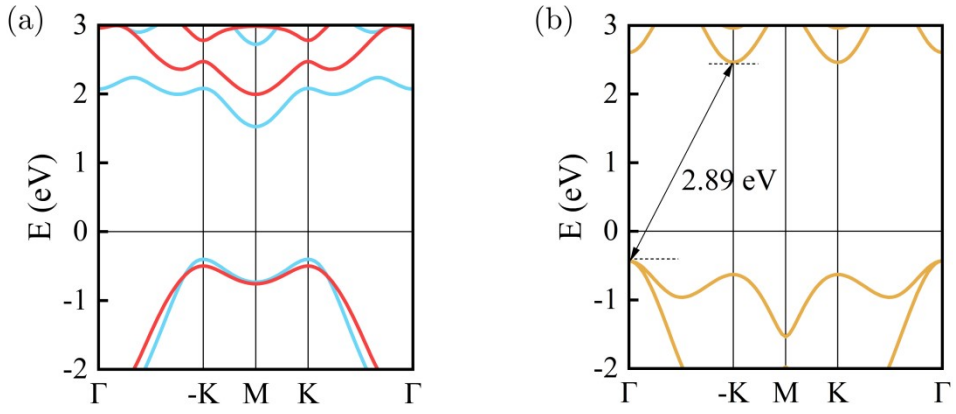

Fig. S1：The band structures of (a) Mn_2ClF and (b) Sc_2CO_2 with HSE06 method, respectively. The blue and red lines represent the spin-up and spin-down bands.

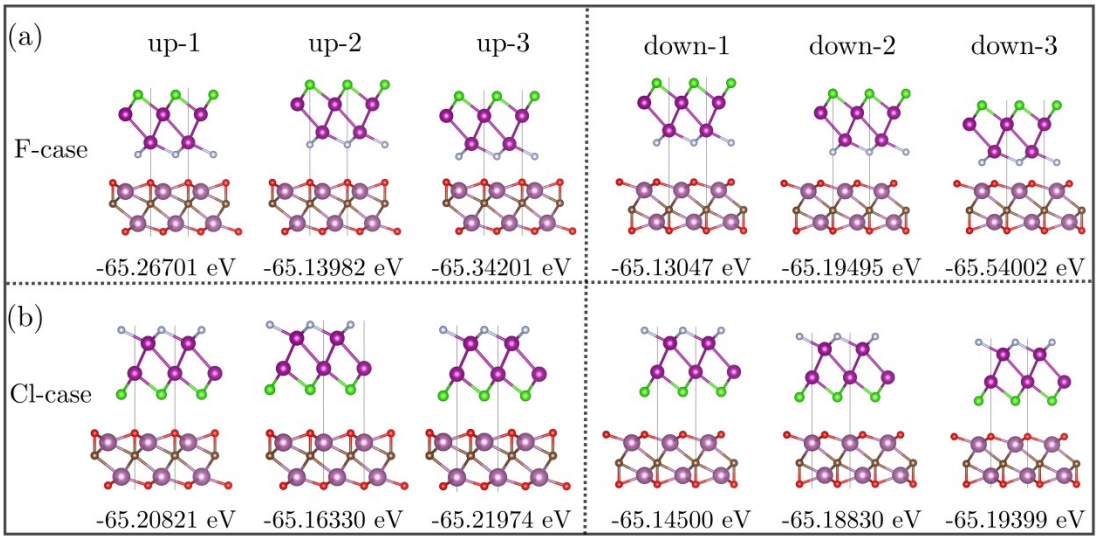

Fig. S2：The Mn_2ClF/Sc_2CO_2 multiferroic vdW heterostructures with different stacking configurations in (a) F-case and (b) Cl-case, respectively.

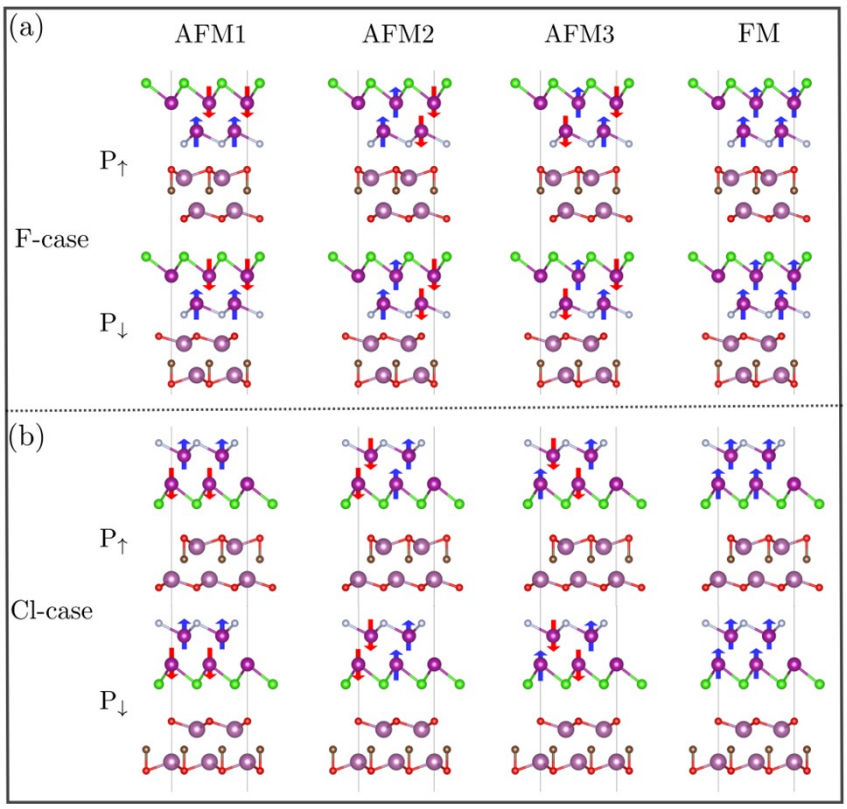

Fig. S3：The different magnetic configurations include AFM1 (A-type AFM), AFM2, AFM3 and FM in (a) F-case and (b) Cl-case, respectively.

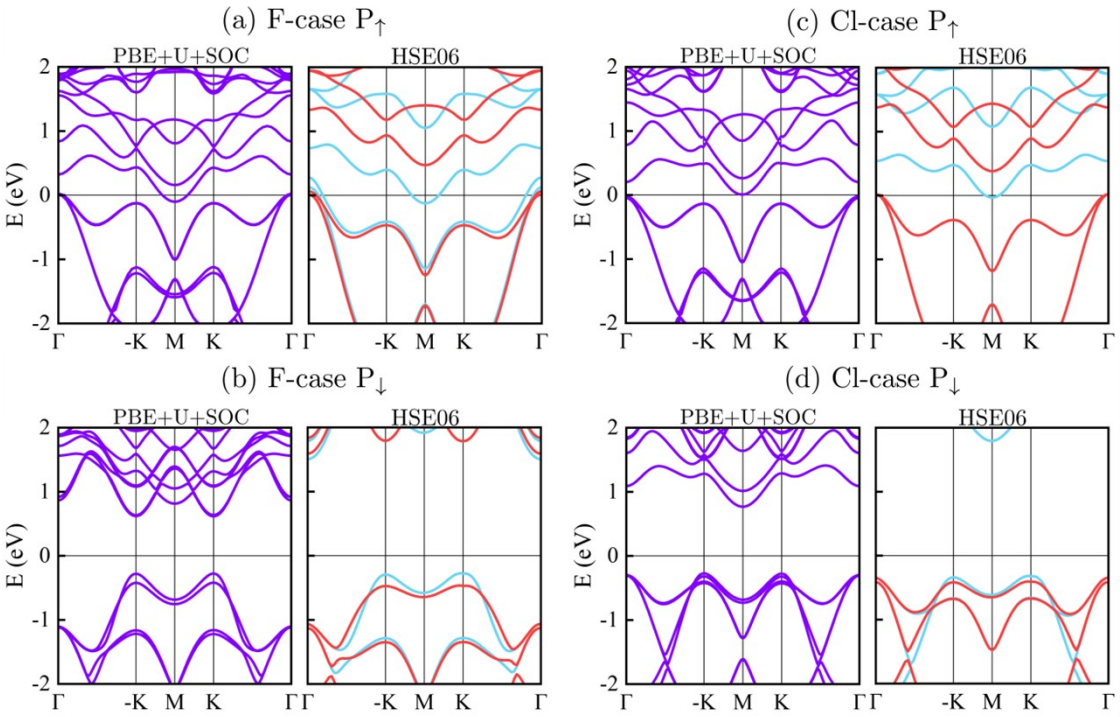

Fig. S4：The band structures of the Mn_2ClF/Sc_2CO_2 heterostructures for $P_{\uparrow}$ and $P_{\downarrow}$ states in (a)(b) F-case and (c)(d) Cl-case with spin-orbit coupling (SOC) effect and HSE06 methods, respectively. Here blue and red symbols denote the contributions from spin-up and spin-down bands, respectively.

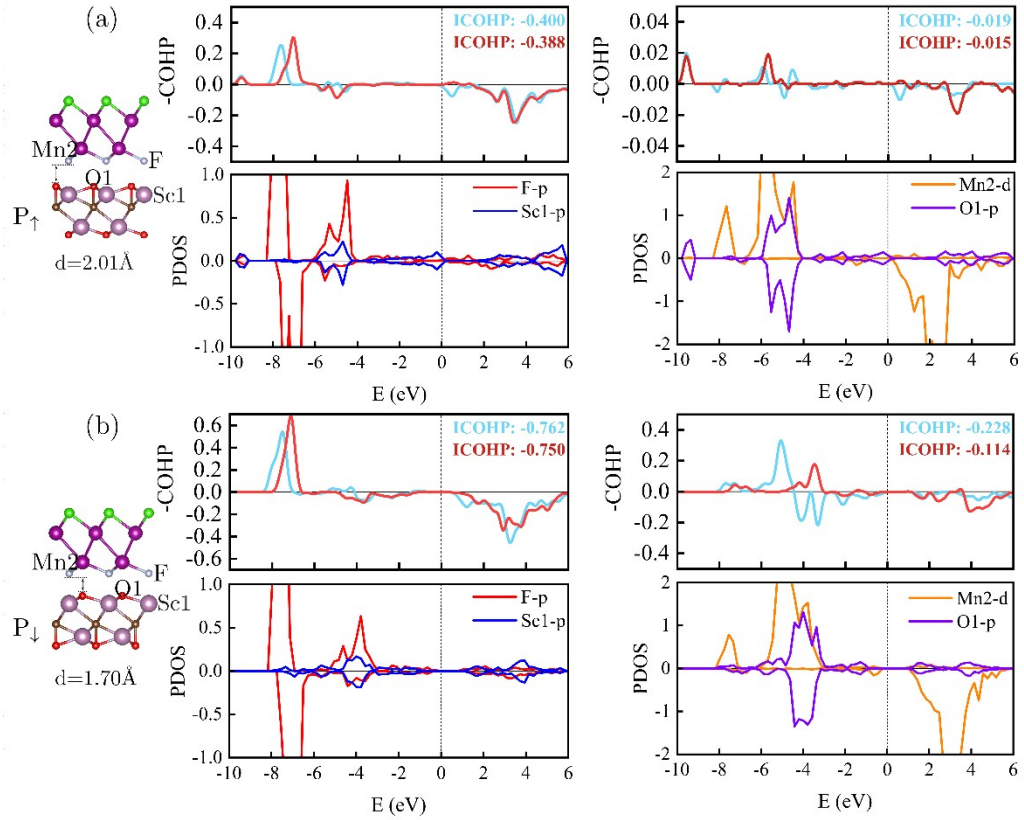

Fig. S5：The spin-polarized projected density of states (PDOS) and the crystal orbital Hamilton population (COHP) of the the interfacial atoms in Mn_2ClF/Sc_2CO_2 (F-case) for (a) $P_{\uparrow}$ and (b) $P_{\downarrow}$ states , respectively.