Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Nonvolatile magnetoelectric coupling in two-dimensional van der Waals sandwich heterostructure $CuInP_2S_6/MnCl_3/CuInP_2S_6$

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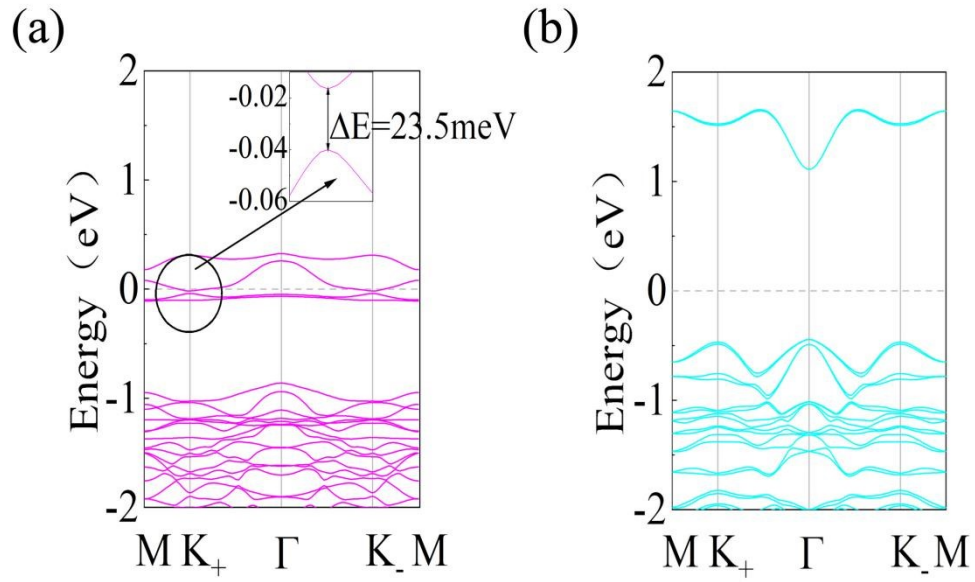

Fig. S1 Band structures of (a) pristine $MnCl_3$ and (b) $CuInP_2S_6$ with SOC. The Fermi level is set to zero.

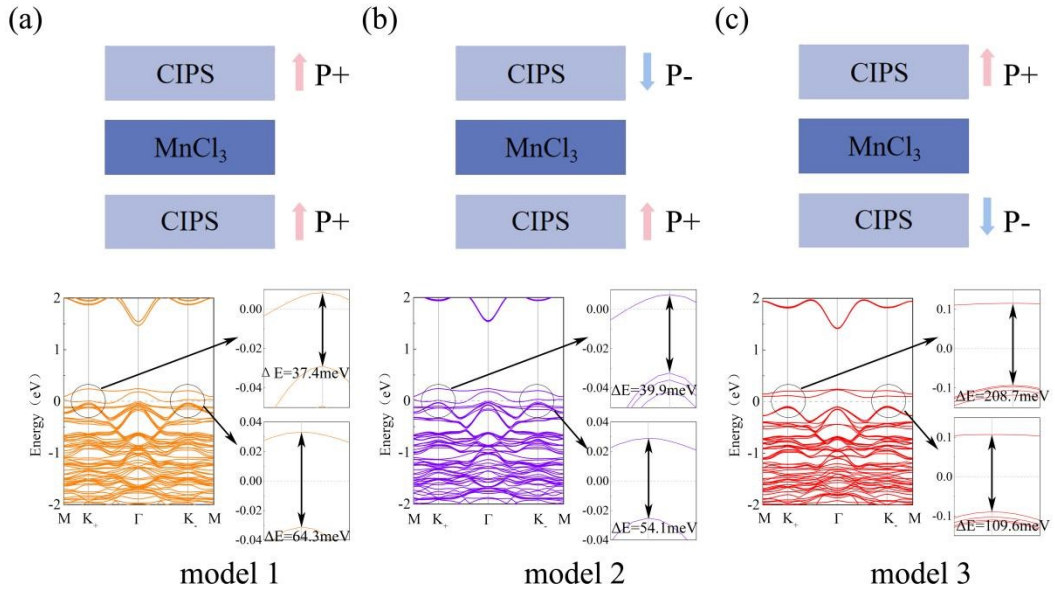

Fig. S2 Band structures of (a) model 1, (b) model 2, and (c) model 3 with SOC. The Fermi level is set to zero. The band-gap at the K_+ and K_- points are marked.

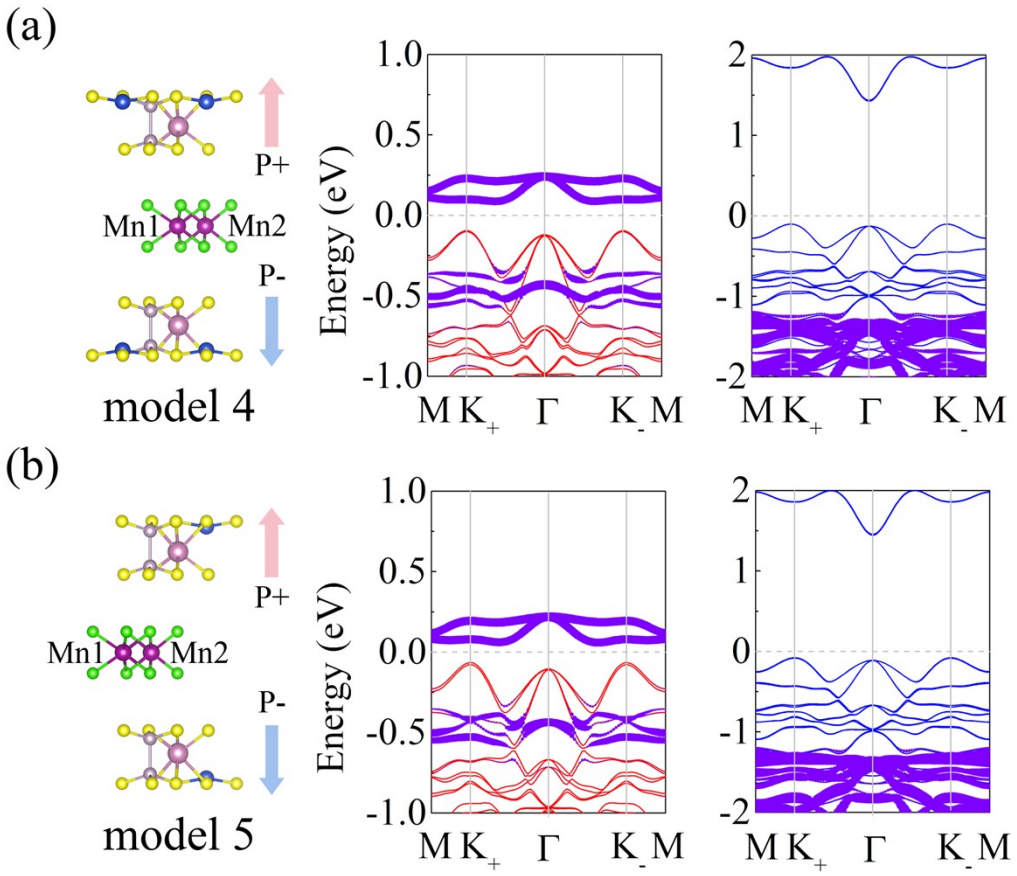

Fig. S3 Atomic and projected band structures of (a) model 4 and (b) model 5 with different stacking arrangements as compared to model 3, without changing the polarized states of $CuInP_2S_6$.

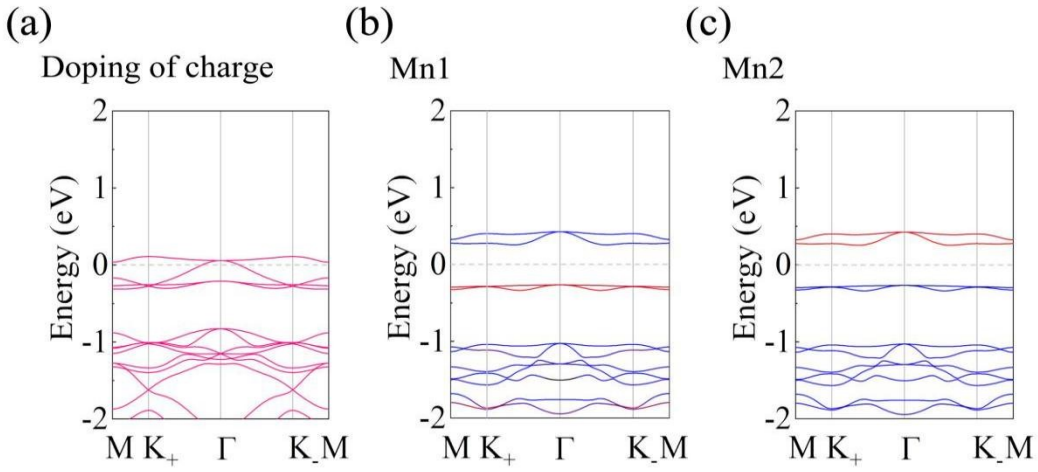

Fig. S4 Band structures of (a) pristine $MnCl_3$ monolayer after electron doping. (b) and (c) are the projected band structures of $MnCl_3$ in the vdW sandwich heterostructure. The red lines denote the contributions from Mn1 and Mn2, as shown in the atomic structure diagram. The Fermi level is set to zero

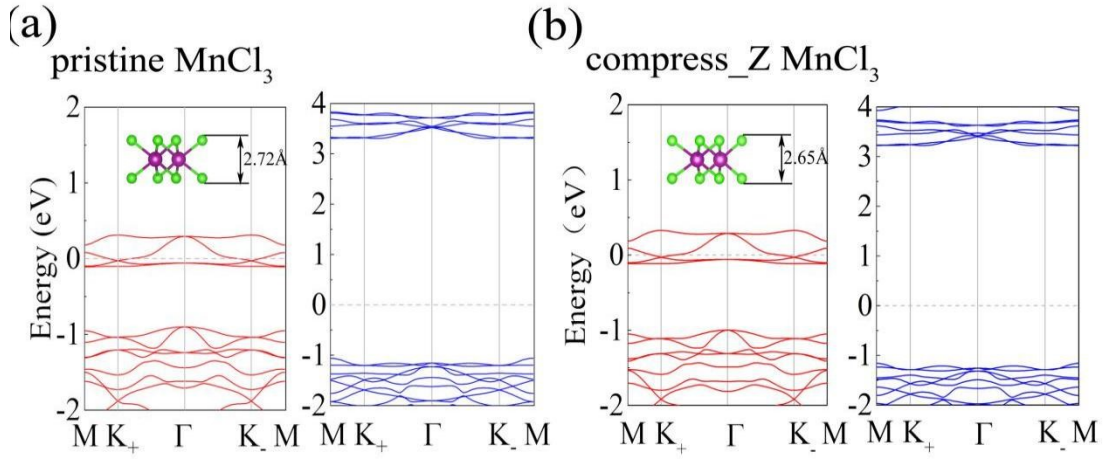

Fig. S5 Electronic band structures of (a) pristine $MnCl_3$ monolayer and (b) isolated $MnCl_3$ with the thickness compress to 2.65 Å.