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Supplementary Information

Theoretical investigation of nonvolatile Electrical Control behavior by ferroelectric polarization switching in two-dimensional $MnCl_3/CuInP_2S_6$ van der Waals heterostructures

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Table S1. Lattice vectors of $MnCl_3/CuInP_2S_6$ heterostructures.

a [Å]	6.2010002136215077	0.0000000000000000	0.0000000000000000
b [Å]	-3.1005001068107538	5.3702237138689561	0.0000000000000000
c [Å]	0.0000000000000000	0.0000000000000000	29.6814002991000017

Table S2. The fractional coordinates of each atom in $MnCl_3$/P↑ $CuInP_2S_6$ heterostructure.

S	0.9950218159465661	0.6426062395755120	0.4580828588801800
S	0.3573937604244881	0.3524155763710541	0.4580828588801800
S	0.6475844236289460	0.0049781840534340	0.4580828588801800
S	0.3432481349086217	0.0234586925278504	0.3448902457958741
S	0.9765413074721496	0.3197894423807570	0.3448902457958741
S	0.6802105576192430	0.6567518650913784	0.3448902457958741
Cl	0.9949357639862565	0.6314663938413753	0.6576594522509940
Cl	0.3685336061586247	0.3634693701448812	0.6576594522509940
Cl	0.6365306298551189	0.0050642360137435	0.6576594522509940
Cl	0.9946438358744023	0.3586483447545852	0.5668409493374150
Cl	0.6413516552454148	0.6359954911198170	0.5668409493374150
Cl	0.3640045088801830	0.0053561641255978	0.5668409493374150
P	0.6666666666666643	0.3333333333333357	0.3621957902770818
P	0.6666666666666643	0.3333333333333357	0.4377279602287430
Mn	0.6666666666666643	0.3333333333333357	0.6123631946991746
Mn	0.3333333333333357	0.6666666666666643	0.6122511351026667
Cu	-0.0000000000000000	-0.0000000000000000	0.4427931098441662
In	0.3333333333333357	0.6666666666666643	0.3946783720547221

Table S3. The fractional coordinates of each atom in $MnCl_3$/P↓ $CuInP_2S_6$ heterostructure.

S	0.9956541860077024	0.6421067179585445	0.6552080165150977
S	0.3578932820414554	0.3535474680491432	0.6552080165150977
S	0.6464525319508568	0.0043458139922979	0.6552080165150977
S	0.3410543853226823	0.0255087952080273	0.5423351132175384
S	0.9744912047919727	0.3155455901146547	0.5423351132175384
S	0.6844544098853452	0.6589456146773180	0.5423351132175384
Cl	0.0132735820988736	0.6447799846319541	0.4335411952554460
Cl	0.3552200153680459	0.3684935974669197	0.4335411952554460
Cl	0.6315064025330804	0.9867264179011266	0.4335411952554460
Cl	0.0128275875559323	0.3709104984761558	0.3429512661513728
Cl	0.6290895015238438	0.6419170890797761	0.3429512661513728
Cl	0.3580829109202239	0.9871724124440678	0.3429512661513728
P	0.6666666666666643	0.3333333333333357	0.5595235483127348
P	0.6666666666666643	0.3333333333333357	0.6349994616356982
Mn	0.6666666666666643	0.3333333333333357	0.3882145389737788
Mn	0.3333333333333357	0.6666666666666643	0.3882880232272887
Cu	0.0000000000000000	-0.0000000000000000	0.6396379278570667
In	0.3333333333333357	0.6666666666666643	0.5909096645750912

Table S4. Total energies of different spin-polarized states, including FM configuration and three typical AFM configurations (Phys. Rev. B, 2018, 97, 094408, AFM-Néel, AFM-stripy, and AFM-zigzag.)

	FM	Néel	stripy	zigzag
$MnCl_3$	-130.83813109	-130.23092055	-130.40502121	-130.62658804
$MnCl_3$/P↑ $CuInP_2S_6$	-319.66450733	-319.03276800	-319.27790273	-319.44384364
$MnCl_3$/P↓ $CuInP_2S_6$	-319.45389657	-319.00639879	-319.16541976	-319.29788037

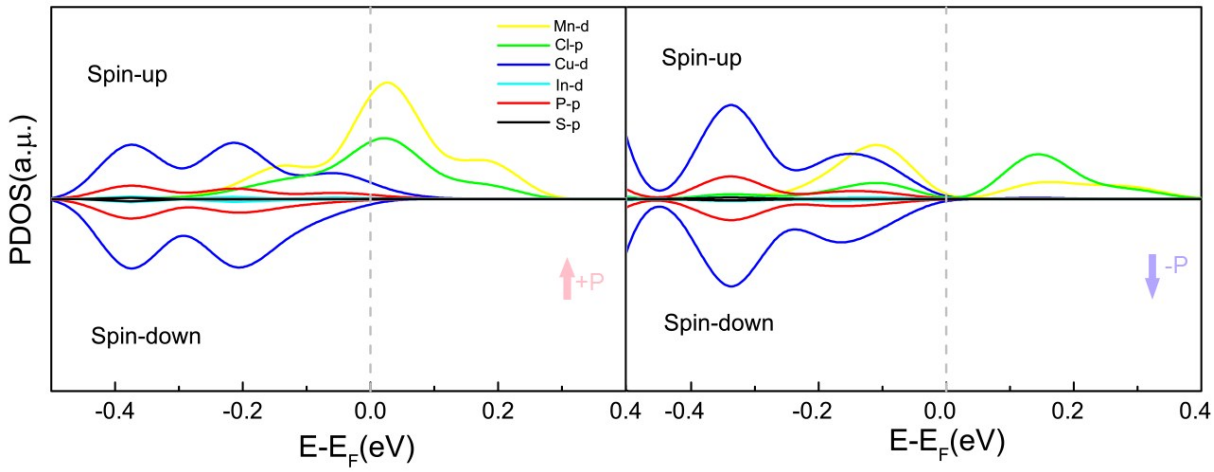

Fig. S1. Spin-resolved PDOS of the atomic orbitals in $MnCl_3$/P↑ $CuInP_2S_6$ and $MnCl_3$/P↓ $CuInP_2S_6$ heterostructures. The Fermi level is set to zero.

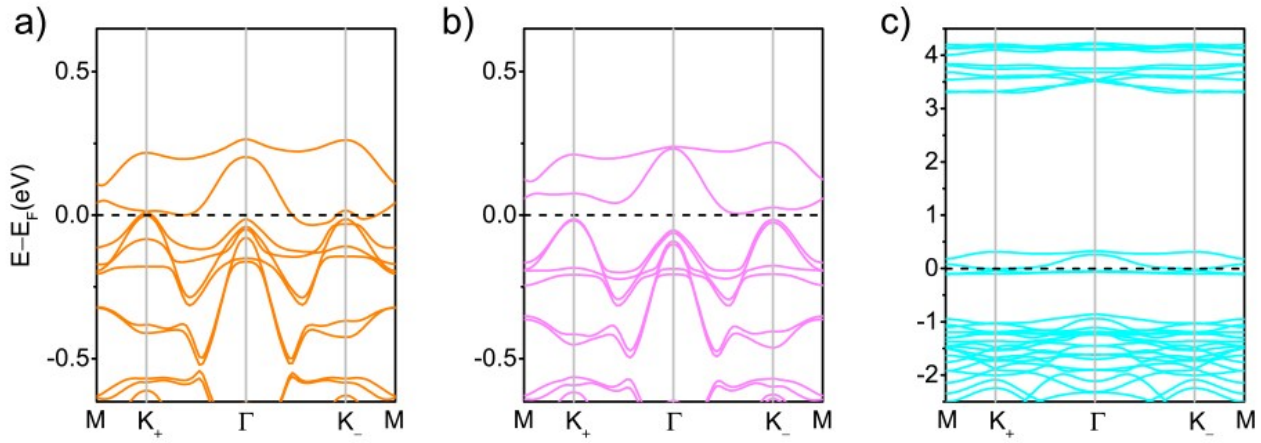

Fig. S2. Electronic band structures of a) $MnCl_3$/P↑ $CuInP_2S_6$, b) $MnCl_3$/P↓ $CuInP_2S_6$, and c) pristine $MnCl_3$ with SOC. The Fermi level is set to zero.