

Supporting information for “The Dirac half-semimetal and quantum anomalous Hall effect in two-dimensional Janus $\text{Mn}_2\text{X}_3\text{Y}_3$ ($\text{X}, \text{Y} = \text{F}, \text{Cl}, \text{Br}, \text{I}$)”

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1. Table SI the different magnetic configuration of the total energy.
2. Figure S1 the total energy fluctuation of the $\text{Mn}_2\text{X}_3\text{Y}_3$ during the MD simulation at 300 K.
3. Figure S2 the phonon dispersion curves of the $\text{Mn}_2\text{Cl}_3\text{Br}_3$.
4. Figure S3 the calculated spin-polarized band structures of $\text{Mn}_2\text{F}_3\text{Br}_3$, $\text{Mn}_2\text{F}_3\text{I}_3$, and $\text{Mn}_2\text{Cl}_3\text{I}_3$.
5. Figure S4 the energy and k contribution of $\text{Mn}_2\text{Cl}_3\text{Br}_3$ to the spin up bands.

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TABLE S1. Different magnetic configuration of the total energy E (meV/cell) (relative to the FM state).

| | FM | AFM-N | AFM-ZZ | AFM-C-I | AFM-C-II | AFM-C-III |
|-------------------------------------|------|--------|--------|---------|----------|-----------|
| $\text{Mn}_2\text{F}_3\text{Cl}_3$ | 0.00 | 295.68 | 340.53 | 381.75 | 521.53 | 428.99 |
| $\text{Mn}_2\text{F}_3\text{Br}_3$ | 0.00 | 314.88 | 428.90 | 572.70 | 428.94 | 610.94 |
| $\text{Mn}_2\text{F}_3\text{I}_3$ | 0.00 | 335.04 | 221.51 | 216.81 | 192.54 | 257.94 |
| $\text{Mn}_2\text{Cl}_3\text{Br}_3$ | 0.00 | 446.40 | 257.06 | 446.08 | 389.98 | 397.44 |
| $\text{Mn}_2\text{Cl}_3\text{I}_3$ | 0.00 | 456.00 | 270.80 | 299.35 | 261.60 | 345.70 |
| $\text{Mn}_2\text{Br}_3\text{I}_3$ | 0.00 | 463.68 | 224.51 | 366.95 | 324.76 | 329.23 |

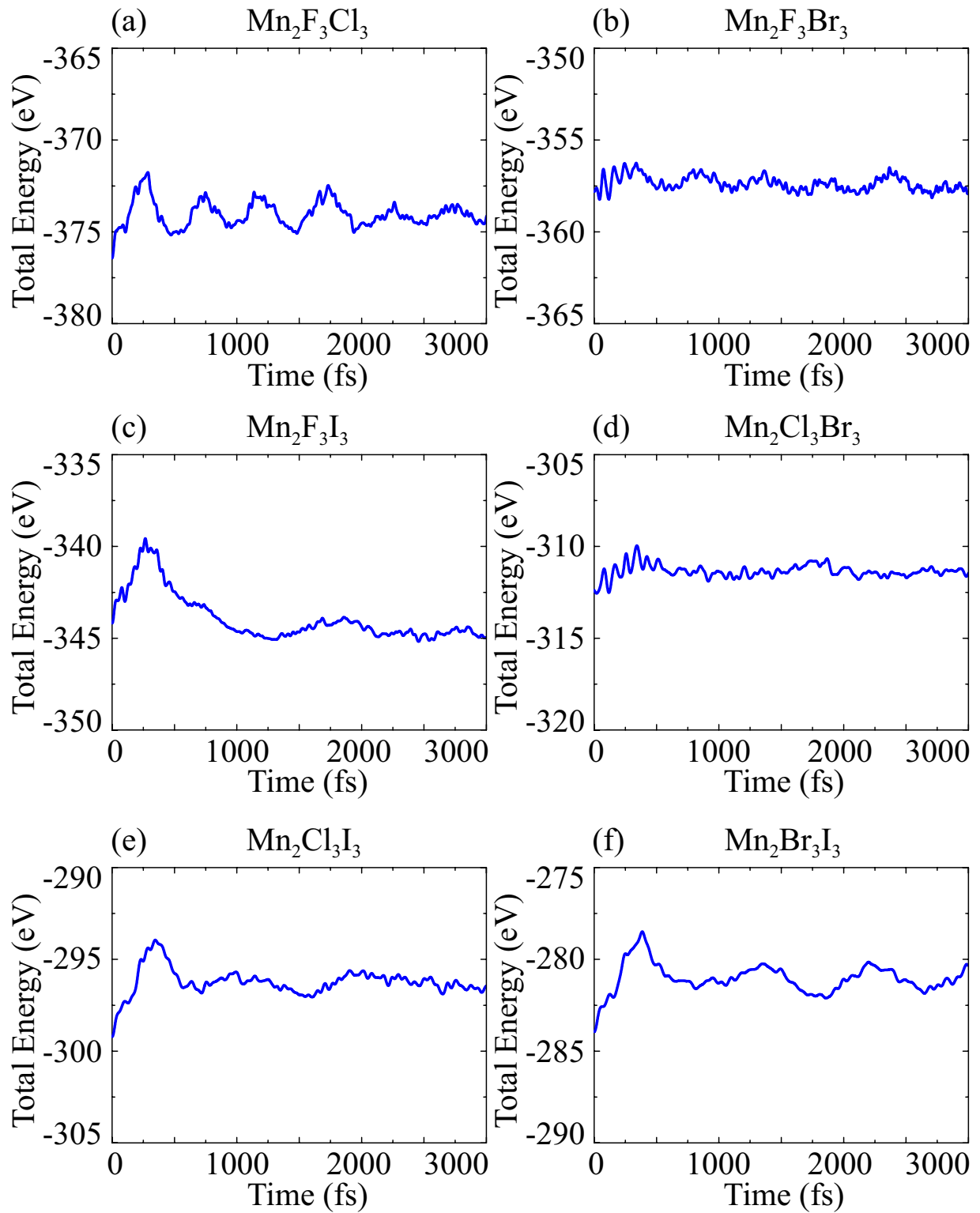


FIG. S1. Total energy fluctuations of the $\text{Mn}_2\text{X}_3\text{Y}_3$ monolayer during 3 ps MD simulation at 300 K.

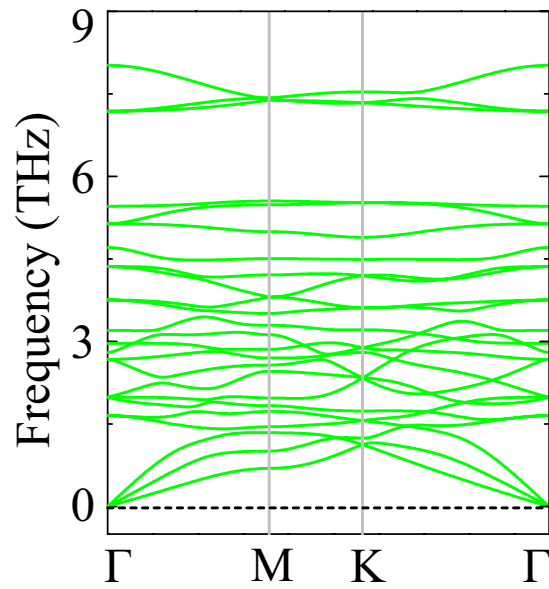


FIG. S2. Phonon dispersion curves of the $\text{Mn}_2\text{Cl}_3\text{Br}_3$.

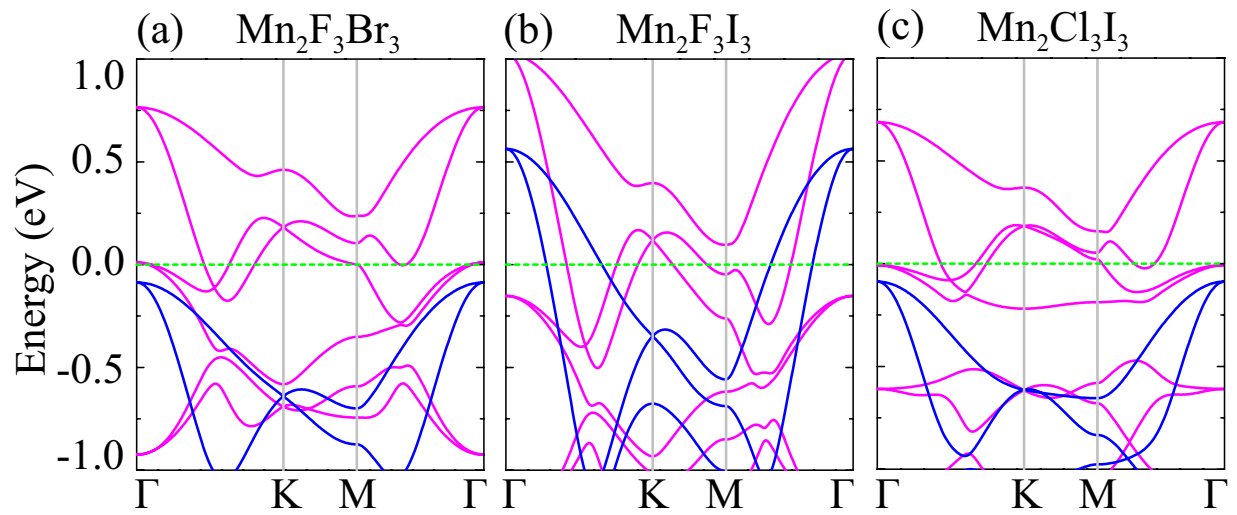


FIG. S3. The calculated spin-polarized band structures of $\text{Mn}_2\text{F}_3\text{Br}_3$, $\text{Mn}_2\text{F}_3\text{I}_3$, and $\text{Mn}_2\text{Cl}_3\text{I}_3$. Spin up and spin down bands are plotted as magenta and blue curves, respectively.

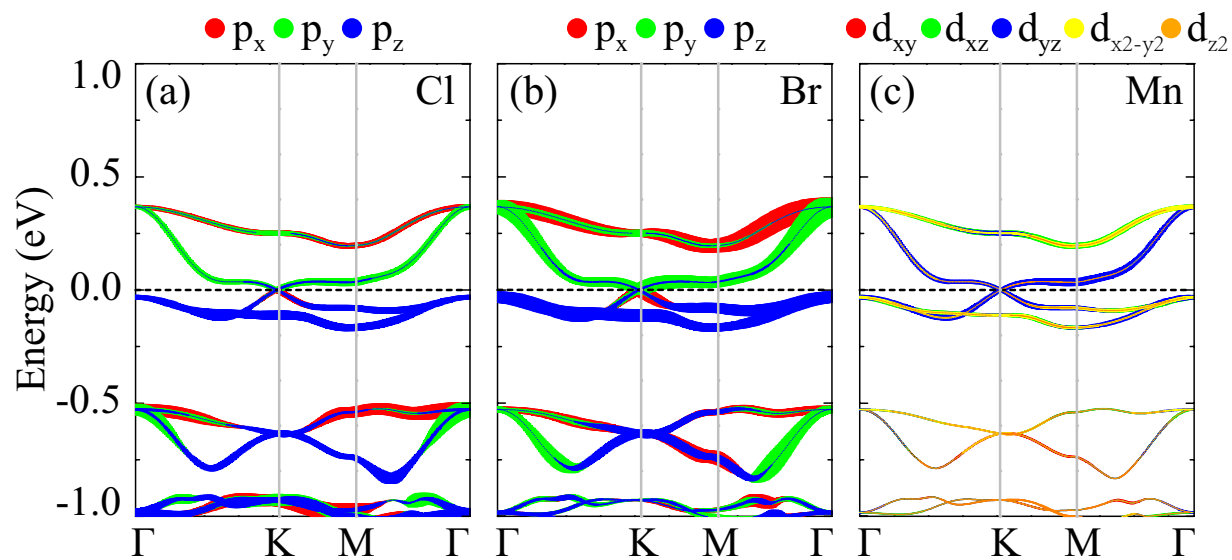


FIG. S4. Energy and k contribution of $\text{Mn}_2\text{Cl}_3\text{Br}_3$ for Cl p-resolved, Br p-resolved and Mn d-resolved to the spin up bands.