New Two-Dimensional Mn-based MXenes with Room-Temperature Ferromagnetism and Half-Metallicity

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1. Comparison of H and T structure

![H-structure vs. T-structure](image)

**Fig. S1.** The relative energy for H and T structure Mn2C monolayer.

![Site 1 and Site 2](image)

**Fig. S2.** Two possible sites for functional atoms/groups, site 1 and site 2 are shown in parts (a) and (b), respectively; top and side views are shown in upper and lower panels, respectively.
2. Structural stability of Mn$_2$CF$_2$ monolayer

To study the thermal stability of the Mn$_2$CF$_2$ MXenes monolayer, the \textit{ab initio} molecular dynamics (AIMD) simulations at 500 K in a canonical ensemble are performed using the Nosé heat bath approach. The phonon frequencies were calculated by using density functional perturbation theory (DFPT) approach as implemented in the PHONOPY code.$^{1, 2}$

![Image of graph showing total potential energy and phonon dispersion curves](image)

**Fig. S3:** (a) Variations of the total potential energy of Mn$_2$CF$_2$ monolayer during \textit{ab initio} molecular dynamics simulations at 500 K. (b) Phonon dispersion curves for Mn$_2$CF$_2$ monolayer.
3. The band structure of Mn$_2$CF$_2$ at HSE06 level.

![Band structure of Mn$_2$CF$_2$](image)

**Fig. S4.** The band structure of Mn$_2$CF$_2$ calculated at the HSE06 level. The red and blue curves represent the spin-up and spin-down channels, respectively.

![Spin charge density](image)

**Fig. S5.** The spin charge density for Mn$_2$C (a) and Mn$_2$CO$_2$ (b) are calculated, respectively.

The red and blue densities represent the spin-up and spin-down, respectively.
FigS6. PDOS of Mn $d$ states (blue, red, and green) and C and O $p$ states for Mn$_2$CO$_2$ (black and brown, respectively) are shown.

Reference
