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

Junjie He,[†] Pengbo Lyu, [†] and Petr Nachtigall*,[†]

[†]*Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, 128 43 Prague 2, Czech Republic*

E-mail: petr.nachtigall@natur.cuni.cz

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1. Comparison of H and T structure

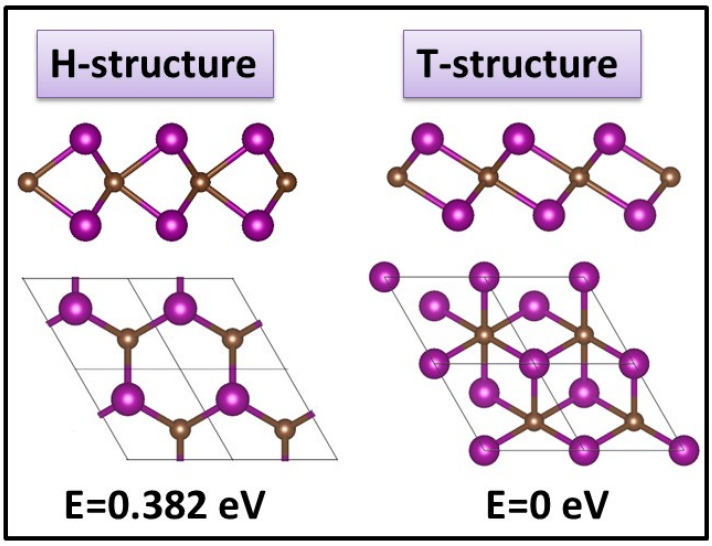


Fig. S1. The relative energy for H and T structure Mn2C monolayer.

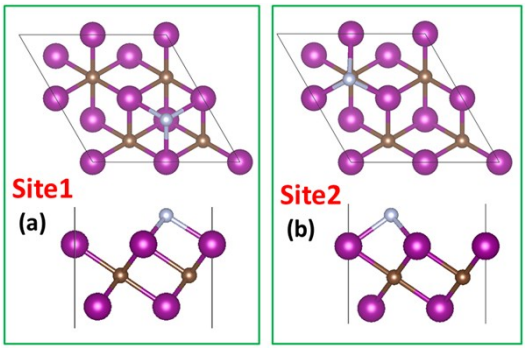


Fig. S2. Two possible sites for functional atoms/groups, site 1 and site 2 are shown in parts (a) and (b), respectively; top and side views are shown in upper and lower panels, respectively.

2. Structural stability of Mn_2CF_2 monolayer

To study the thermal stability of the Mn_2CF_2 MXenes monolayer, the *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]

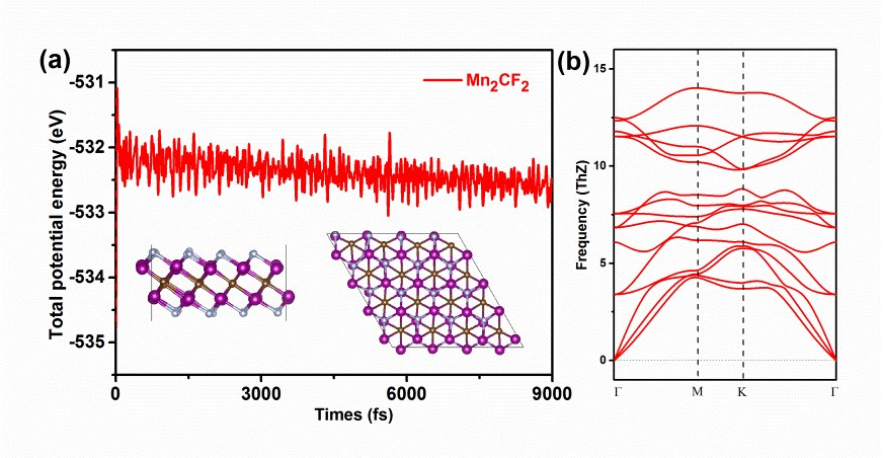


Fig. S3: (a) Variations of the total potential energy of Mn_2CF_2 monolayer during *ab initio* molecular dynamics simulations at 500 K. (b) Phonon dispersion curves for Mn_2CF_2 monolayer.

3. The band structure of Mn_2CF_2 at HSE06 level.

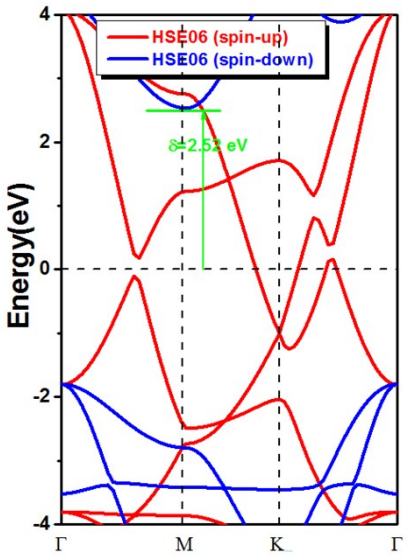


Fig. S4. The band structure of Mn_2CF_2 calculated at the HSE06 level. The red and blue curves represent the spin-up and spin down channels, respectively.

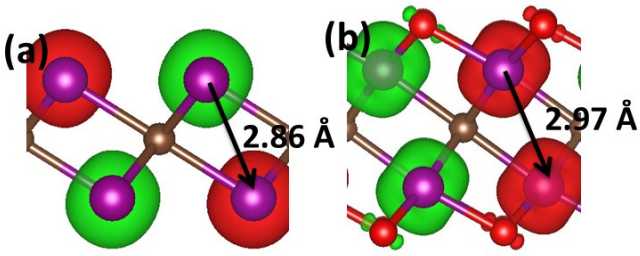
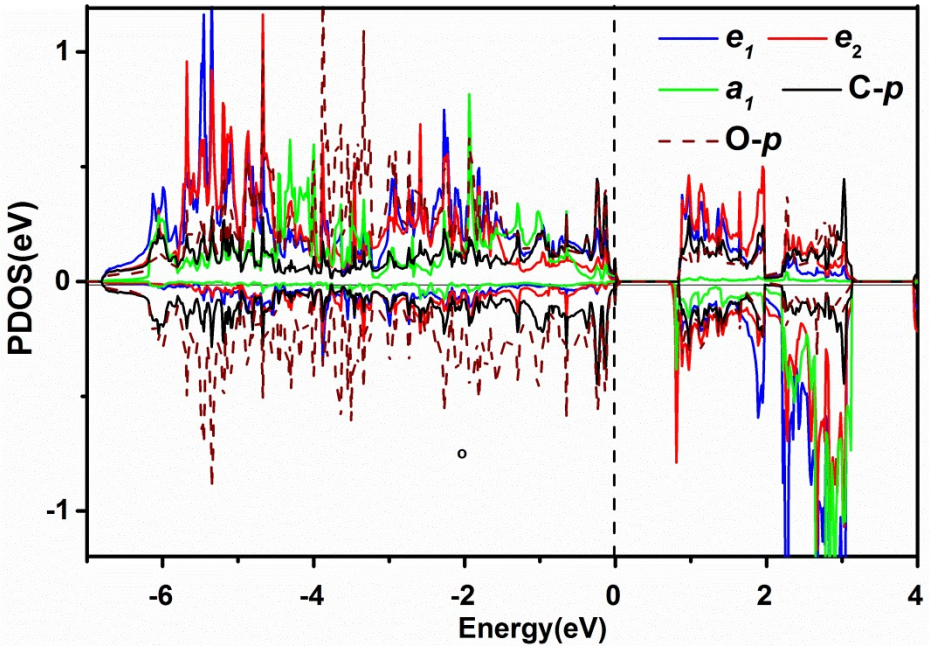


Fig. S5. The Spin charge density for Mn_2C (a) and Mn_2CO_2 (b) are calculated, respectively. The red and blue densities represent the spin-up and spin down, respectively.



FigS6. PDOS of Mn *d* states (blue, red, and green) and C and O *p* states for Mn_2CO_2 (black and brown, respectively) are shown.

Reference

[1] K. Parlinski, Z. Q. Li, Y. Kawazoe, *Phys. Rev. Lett*., 1997, **78**, 4063.

[2] A. Togo, O. Fumiyasu, T. Isao, *Phys. Rev. B,* 2008, **78**(13), 134106.