Supporting Information

Modulation of the Electronic and Magnetic Properties of an $MnCrNO_2$ Ferromagnetic Semiconductor MXene

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Supplementary Note 1: Antiferromagnetic Configurations

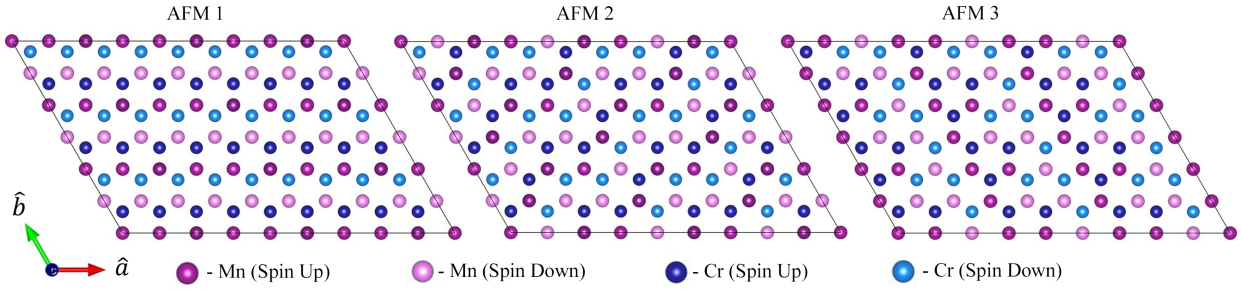
We have found three possible antiferromagnetic configurations considering $3 \times 2 \times 1$ supercell for the MnCrNO2 MXene, which named AFM 1, AFM 2, AFM 3. Each MXene has six layers of both Mn and Cr layers.

AFM 1: In this configuration, each atom along the $\hat{a}$ direction has identical spin orientation. However, the neighboring atoms along the $\hat{b}$ direction have opposite spin orientations.

AFM 2: In this configuration, each atom along the $\hat{b}$ has an opposite spin orientation. Along the $\hat{a}$ direction, atoms follow a repeated pattern where every other layer alternates between two spin-up atoms followed by one spin-down atom, or one spin-up atom followed by two spin-down atoms.

AFM 3: This configuration is almost like AFM 2 with one key difference. In the $\hat{b}$ direction, in every other layer features neighboring atoms with either identical spins or opposite spin orientations alternately.

The figure 1 indicates the expanded supercell of $9 \times 6 \times 1$ for better clarity. These configurations are crucial to understand the magnetic properties of the MXene.



Supplementary Figure 1: Possible antiferromagnetic arrangements with various spin configurations

Supplementary Note 2: Atomic Magnetic Moments

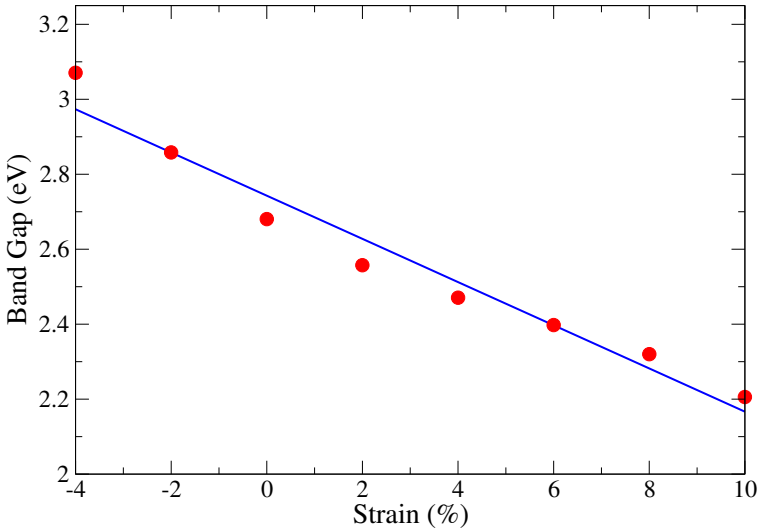
Supplementary Table 1 shows the approximated magnetic moment of each element of $MnCrNO_2$ MXene. Mn and Cr have large positive magnetic moments, indicating the presence of unpaired electrons. These elements contribute significantly to the overall magnetic behavior, as their magnetic moments can align in the same direction within the material. N and O have small negative magnetic moments. In ferromagnetic materials, these negative values could indicate the presence of magnetic interactions that slightly oppose the main magnetic alignment but are overwhelmed by the positive moments of Mn and Cr.

Supplementary Table 1: Magnetic moment of each element of $MnCrNO_2$ MXene.

Element	Magnetic Moment (μ_B)
Mn	3.44
Cr	2.98
N	-0.22
O	-0.12

Supplementary Note 3: Hybrid Functional Calculations

Supplementary Fig. 2 illustrates the band gap as a function of strain, calculated using the HSE06 hybrid functional. This functional is commonly employed in density functional theory (DFT) to achieve more accurate electronic structure predictions by mitigating self-interaction errors. The linear trend in the data is represented by the best-fit line, determined via the least squares method, which follows the equation $y = -0.0576x + 2.743$ with an R^2 value of 0.96. These findings suggest that the band gap can be accurately predicted by this linear relationship.



Supplementary Figure 2: (a) The band gap of Mn_2NO_2 MXene under biaxial strain based on the HSE06 hybrid functional calculations. The straight lines represent the best fit line found by the least square technique.

Supplementary Note 4: Ground State Structure

The following CIF file contains the ground state structure of Mn_2NO_2 MXene.

```
# CIF file

data_findsym-output

_symmetry_space_group_name_H-M 'P 3 m 1'
_symmetry_Int_Tables_number 156

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_cell_length_b       2.98300
_cell_length_c      24.12800
_cell_angle_alpha   90.00000
_cell_angle_beta    90.00000
_cell_angle_gamma  120.00000

loop_
_space_group_symop_operation_xyz
x,y,z
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-x+y,-x,z
-x+y,y,z
-y,-x,z
x,x-y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mn1 Mn   0.00000   0.00000   0.48877   1.00000
Cr1 Cr   0.33333   0.66667  -0.40542   1.00000
N1  N    0.66667   0.33333  -0.46413   1.00000
O1  O    0.33333   0.66667   0.44996   1.00000
O2  O    0.00000   0.00000  -0.36918   1.00000

# end_of_file
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