First-Principles Study of the Ferromagnetic Properties of Cr\textsubscript{2}CO\textsubscript{2} and Cr\textsubscript{2}NO\textsubscript{2} MXenes

Zhiyun Tan,*, Zhenxing Fang, Baihai Li,* and Youchang Yang

ABSTRACT: Massive attention has been paid to MXenes due to their intriguing properties and potential diverse applications. Extensive studies using first-principles calculations on the electronic structures of MXenes Cr\textsubscript{2}CO\textsubscript{2} and Cr\textsubscript{2}NO\textsubscript{2} were performed in this paper. Based on the accurate Heyd–Scuseria–Ernzerhof (HSE) calculations, Cr\textsubscript{2}CO\textsubscript{2} is clarified to be a ferromagnetic semiconductor; meanwhile, Cr\textsubscript{2}NO\textsubscript{2} is a half-metallic material, which is consistent with previous results. In particular, by analyzing the contribution of the orbitals to the band structures and density of states, the basic mechanism of ferromagnetism was analyzed in detail. Our theoretical work might promote the spintronics study and application of Cr-contained MXenes.

INTRODUCTION

In the recent decade, single-layer free-standing atomic crystal graphene, exfoliated mechanically from its bulk structure,\textsuperscript{1,2} opens up a new area of two-dimensional (2D) materials in the field of material research, where BN, MoS\textsubscript{2},\textsuperscript{3} and ZnO monolayers\textsuperscript{4} and other two-dimensional materials are successfully synthesized. Two-dimensional transition metal carbides and carbonitrides denoted MXenes have drawn massive attention due to their intriguing properties and potential diverse applications.\textsuperscript{5} Recent studies indicate that MXenes are derived by selective etching using hydrofluoric acid from MAX phases.\textsuperscript{6,7} During the process of synthesis, the surfaces of bare MXenes are chemically active and are terminated by some functional groups such as oxygen (O), fluorine (F), and hydroxyl (OH) in most cases, dramatically causing variable properties in electronic structure, geometrical mechanics,\textsuperscript{8} thermoelectricity,\textsuperscript{9} thermal stability,\textsuperscript{10} carrier mobility,\textsuperscript{11} and other aspects. Thus, the MXene family has a large number of applications such as lithium-ion batteries,\textsuperscript{12} electrochemical capacitor electrodes,\textsuperscript{13} capacitors,\textsuperscript{14} field-effect transistors,\textsuperscript{15} and so on.

Note that the magnetic properties of the MXene family are also an attractive topic.\textsuperscript{16–19} The magnetism of F- and OH-functionalized Cr-based MXenes [Cr\textsubscript{2}CF\textsubscript{2} and Cr\textsubscript{2}C(OH)\textsubscript{2}] were first reported by Khazaei et al.\textsuperscript{20} basing on their density functional theory (DFT) calculations, while the O-functionalized Cr\textsubscript{2}C (Cr\textsubscript{2}CO\textsubscript{2}) is a nonmagnetic material; however, the authors did not explain why the magnetic moments of the transition metal Cr atoms of Cr\textsubscript{2}CO\textsubscript{2} have vanished. Interestingly, Si et al.\textsuperscript{21} predicted the bare Cr\textsubscript{2}C MXene to be half-metallic but did not mention the magnetic properties of Cr\textsubscript{2}CO\textsubscript{2}, whereas the F-, OH-, chlorine (Cl)-, and hydrogen (H)-functionalized Cr\textsubscript{2}C were calculated to be antiferromagnetic semiconductors. It seems that the magnetism of Cr\textsubscript{2}CO\textsubscript{2} MXene is in controversy. On the other hand, the nitride MXene is a magnetic material.\textsuperscript{17} Therefore, investigation of the magnetic properties and the intrinsic mechanism of Cr-based MXene Cr\textsubscript{2}CO\textsubscript{2} and Cr\textsubscript{2}NO\textsubscript{2} is important and necessary.

In our work, DFT + U calculations were first performed to obtain the energetically favorable structures of Cr\textsubscript{2}CO\textsubscript{2} and Cr\textsubscript{2}NO\textsubscript{2}. To improve the accuracy and authenticity of our calculations, accurate Heyd–Scuseria–Ernzerhof (HSE) screened Coulombic hybrid density functional\textsuperscript{22–24} methods were used then to examine the magnetism of these two MXenes and magnetic coupling of Cr atoms. The band structures of Cr\textsubscript{2}CO\textsubscript{2} and Cr\textsubscript{2}NO\textsubscript{2} were obtained by the extensive studies, from which a magnetic semiconductor feature for Cr\textsubscript{2}CO\textsubscript{2} MXene and a half-metallicity feature for Cr\textsubscript{2}NO\textsubscript{2} MXene were unfolded. Finally, the orbital contribution of each atom to the band structure and the spin density distribution of states were analyzed to uncover the nature of electronic properties.

Received: July 1, 2020
Accepted: September 18, 2020
Published: October 1, 2020
RESULTS AND DISCUSSION

Single-layer MXene Cr$_2$C/Cr$_2$N is a centered honeycomb (T) structure with the C$_6$v symmetry, in which the 2D hexagonal lattice of C/N atoms is sandwiched between two layers of hexagonal lattices of positively charged Cr atoms. There are four possible sites for oxygen adsorption on Cr$_2$C/Cr$_2$N, as shown in Figure 1. The O atoms locating right above both the structures.

Figure 1. Side view of four possible crystal structures of oxygen-functionalized Cr-based MXene. (a) Both O atoms on Cr atoms; (b) both O atoms above the opposite Cr atoms; (c) one O atom above C(N) atom and the other O atom above the opposite Cr atom; and (d) both O atoms above the C(N) atom. The blue and red balls denote Cr and O atoms, respectively. C or N atoms are shown by gray balls.

Cr atoms are represented by Model 1 and those at the hollow sites of adjacent carbon atoms are shown in Model 2. In Model 3, one O atom sits above the C atom and the other O atom sits at the opposite side on the hollow site of the other carbon atom. The O atoms placed on the top of the C atoms are denoted as Model 4. DFT + U calculations were adopted first to quickly determine the most preferential location of the functional O atoms. The energies per unit cell listed in Table 1 clearly indicate that the most stable structure of Cr$_2$CO$_2$ and Cr$_2$NO$_2$ MXene is model 4 and model 2, respectively.

Interestingly, the HSE-calculated results show that the energy of the ferromagnetic (FM) state is 0.54 eV per unit cell lower than that of the antiferromagnetic (AFM) ordering for Cr$_2$CO$_2$ and Cr$_2$NO$_2$ indicating that the ground state of Cr$_2$CO$_2$ is in ferromagnetic ordering. In the AFM configuration, the values of the magnetic moments are 0.31 μB for each Cr atom, and the HSE band gap is calculated to be 0.46 eV.

Moreover, Cr$_2$NO$_2$ also energetically prefers to be ferromagnetic with 0.78 eV per unit cell lower than the total energy of Cr$_2$NO$_2$ in AFM ordering, and each Cr atom has a magnetic moment of 2.67 μB which is comparable to other theoretical results. In the AFM configuration of Cr$_2$NO$_2$, the values of the magnetic moments are 0.43 μB for each Cr atom, and the band gap is 0.52 eV, based on the HSE calculations. To identify the magnetic interactions of the Cr atoms of the MXenes, a 2 × 2 supercell was built for further verification. Figure 2a shows FM coupling ordering, and Figure 2b,c are two possible configurations of AFM ordering, respectively. The energies of the AFM1 and AFM2 configurations of Cr$_2$CO$_2 $ were 0.52 and 0.19 eV/u.c. (unit cell) higher than that of its FM ordering; similarly, the energies of the AFM1 and AFM2 configurations of Cr$_2$NO$_2$ were calculated to be 0.68 and 0.26 eV/u.c. higher than that of its FM ordering, respectively. The exchange interactions between the different magnetic orderings can be conveniently investigated using the Heisenberg model with the nearest- and next-nearest-neighbor coupling parameters $J_i$ and $J_j$:

$$ H = -\sum_{i,j} S_i \cdot S_j - \sum_{i,k} S_i \cdot S_k $$

where $S_i$ is the net spin at the Cr site, $(i,j)$ and $(k,l)$ are the nearest and next-nearest site pairs, respectively. On the basis of this model, the energy difference between FM and AFM$_1$ is $3E_{AFM1} - E_{FM} = 245\frac{\mu B^2}{\text{cell}}$, while the energy difference between FM and AFM$_2$ is $E_{AFM2} - E_{FM} = 125\frac{\mu B^2}{\text{cell}}$. Thus, the exchange coupling parameters are calculated to be $J_1 = 1.54$ meV and $J_2 = 2.16$ meV for Cr$_2$NO$_2$, as well as $J_1 = 1.94$ meV and $J_2 = 3.16$ meV for Cr$_2$CO$_2$, respectively. Both exchange parameters are positive, indicating that the FM phase is the favorable coupling configuration for both Cr$_2$CO$_2$ and Cr$_2$NO$_2$. The band structures of Cr$_2$CO$_2$ and Cr$_2$NO$_2$ MXenes calculated by the HSE method are shown in Figure 4a,b, respectively. As for Cr$_2$CO$_2$, a p-type semiconductor feature is presented in the spin-up channel and an intrinsic semiconductor character appears in the spin-down channel, indicating that Cr$_2$CO$_2$ is a ferromagnetic semiconductor. In the spin-up channel, the conduction band minimum (CBM) is located at the K point, while the valence band maximum (VBM) remains between the G and K points of the reciprocal space with a band gap of 0.55 eV. At another aspect, the CBM is at the M point and the VBM is at the G point in the spin-down channel with a band gap of 2.19 eV.
The electronic structure of Cr$_2$NO$_2$ shows a striking half-metallic feature, where a metallic character was presented in the spin-up channel and a large-gap semiconductor character was shown in the spin-down channel, respectively. The half-metallic gap, defined as the difference between the valence band maximum of the spin-down band and the Fermi level, is calculated to be 0.99 eV, suggesting that electrons transported near the Fermi level are virtually 100% spin-polarized even when Cr$_2$NO$_2$ is under a relatively large external voltage bias.

The bare Cr$_2$C MXene has been reported to be a half-metallic material, but the almost inevitable existence of functional groups in the process of synthesis increases the difficulty in synthesizing Cr$_2$C MXene with a higher spin-polarization. This difficulty is illustrated in Figure 6, which shows the orbital contribution of the atoms of Cr$_2$NO$_2$ to the band near the Fermi level. The size of the symbols can intuitively reflect the contribution weight of the different orbitals. The spin-polarized calculations were performed in the HSE method: (a) spin-up and (b) spin-down.
preparing bare Cr$_2$C MXene in an experimental environment. In contrast to previous work, Cr$_2$NO$_2$ was suggested to be a good candidate to be realized in experiments and promising applications in the spintronic field. Unlike the half-metallicity property of graphene nanoribbons, $^{17}$ boron nitride nanoribbons, $^{18}$ and MoS$_2$ nanosheets $^{19}$ induced by external factors, the half-metallic character of Cr$_2$NO$_2$ MXene is intrinsic, which is of great significance for the spintronic research of 2D materials.

For further investigation of the spin-polarized electronic structure, the components of the band structures were extensively analyzed. The contribution of different orbitals of each atom to the spin-polarized bands at the vicinity of the Fermi level for Cr$_2$CO$_2$ and Cr$_2$NO$_2$ is displayed in Figures 5 and 6, respectively. The components with a predominant orbital contribution to every band were presented at any wave vector, while the minor contributing components were omitted. For the spin-up channel of Cr$_2$CO$_2$ (Figure 5a), the valence band is primarily determined by the $d_{zx}$ and $d_{zy}$ orbitals of the two Cr atoms, while the contribution from the $p_z$ orbital of C and the $p_y$ orbital of two O atoms is less remarkable. Furthermore, the states of the CBM locating at the K point are mainly comprised of the $d_{so}$ orbital of the two Cr atoms and the $p_y$ orbital of two O atoms, while the contributions from the C atom are very subtle. For the spin-down band structures of Cr$_2$CO$_2$ (Figure 5b), the $d_{yz}$ orbital of the Cr1 atom, $p_y$ and $p_x$ orbitals of the C atom, as well as the $p_z$ orbital of O atoms made the most contribution to the valence band and the VBM mainly roots in the $p_x$ orbital of the C atom. The different sizes of the symbols at the CBM manifest that the $p_y$ orbitals of C and O atoms are the predominant contributors and the proportions from Cr atoms are negligible.

The spin-polarized band structures of Cr$_2$NO$_2$ are shown in Figure 6. Clearly, the Fermi level is crossing the spin-up valence band (Figure 6a), resulting in the electrons in this channel to exhibit metallic behavior. The component analysis indicates that the valence band mainly consists of the $d_{yz}$ orbitals of the two Cr atoms with a small proportion from the $p_z$ orbitals of the two O atoms, as well as the $p_x$ and $p_y$ orbitals of the C atom. Furthermore, the composition of the spin-up conduction band is much complicated, where the $d_{xy}$ and $d_{x^2−y^2}$ orbitals of the two Cr atoms make the major contributions, followed by the $p_y$ and $p_z$ orbitals of the two O atoms. The component-projected spin-down band structures exhibit an intrinsic semiconductor character (Figure 6b). The $p_z$ orbital of the O2 atom makes a major contribution to the valence band along the high-symmetry M−G axis, followed by the $d_{z^2}$ of Cr1, $d_{yz}$ of Cr2, and $p_z$ of C and O1 atoms. The valence band along the G−K axis is therefore mainly determined by the $p_y$ and $p_z$ orbitals of the C atom with a smaller proportion from the $p_x$ orbitals of the two O atoms, while the contribution from the Cr atoms is negligible. Nevertheless, the conduction band in the spin-down channel is mainly determined by the hybridized 3d orbitals of the Cr atoms.

The spin-polarized total and projected densities of states (DOS) of Cr$_2$CO$_2$ and Cr$_2$NO$_2$ are presented in Figure 7. In agreement with the band structures, the DOS in Figure 7a,d indicates that Cr$_2$CO$_2$ and Cr$_2$NO$_2$ are the ferromagnetic materials, which is mainly originated from the splitting of the 3d orbitals of Cr atoms. The Cr atoms of Cr$_2$CO$_2$ and Cr$_2$NO$_2$ are both in the C$_6h$ triangular crystal field. Thus, the 3d orbitals are degenerated to be two double generate $e_1$ ($d_{xy}$ and $d_{yz}$) and $e_2$ ($d_{xy}$ and $d_{x^2−y^2}$) orbitals and a single $a$ ($d_{z^2}$) orbital. Indeed, the DOS of the degenerate orbitals shown in Figure 7b,c,e,f are almost overlapping around their main peaks. Nevertheless, an important discrepancy between the two MXene materials is that the valence states of the two Cr cations of Cr$_2$CO$_2$ is +4, but the values of the two Cr atoms of Cr$_2$NO$_2$ should be +3 for one Cr cation and +4 for the other one, due to the valence state of the C anion of Cr$_2$CO$_2$ is −4, while the value for N of Cr$_2$NO$_2$ is −3. Based on the lowest energy principle (Hund’s rule), the rest two valence electrons of each Cr atom in Cr$_2$CO$_2$ are almost locating at the spin-up $e_2$ and $a$ orbitals. Due to the large exchange splitting of Cr 3d orbitals, the spin-down channels of $e_2$ and $a$ are significantly shifted upward to be in the range of 1−5 eV, resulting in semiconductor behavior with a band gap of about 2.1 eV between the slightly occupied Cr $d_{z^2}$ and unoccupied Cr $d_{x^2−y^2}$ orbitals. As compared with Cr$_2$CO$_2$, the partial DOSs of Cr atoms in Cr$_2$NO$_2$ are much different. The results are presumably explained as a result of the different electron distributions of the Cr atoms (+4, +4) in Cr$_2$CO$_2$ from that of the Cr atoms (+3, +4) in Cr$_2$NO$_2$. As shown in Figure 7e,f, the strong spin splitting in the spin-up 3d orbitals of Cr atoms pushes down the $d_{x^2−y^2}$ orbitals to a lower energy region, while it shifts the $d_{yz}$ upward and leads the orbital to be partially above the Fermi level, showing metallic character. A large energy gap in the spin-down DOS represents semiconductor behavior.
The magnetic exchange interactions in the Cr$_2$CO$_2$ and Cr$_2$NO$_2$ monolayers mainly originate from two mechanisms: (i) the superexchange ferromagnetism between the nearest intralayered Cr atoms via the outmost oxygen atom in-between (e.g., Cr$_{-}$O$^-$−Cr$_{+}$). According to the Hund’s rule, the electron p’ hopping from O$^{2-}$ onto the less-than-half-filled orbitals of Cr$_{±}$ is aligned parallel to the 3d electrons, e.g., spin-up. Furthermore, the p’-paired electron p” (spin down) transfer from O$^{2-}$ to the 3d orbitals of Cr$_{±}$ with the unchanged spin direction, which is determined by the negative exchange integral between O$^-$−p” and Cr$_{±}$−3d orbitals, leading the 3d electrons on Cr$_{±}$ to spin-up. (ii) The competition between ferromagnetic superexchange and antiferromagnetic interactions between the nearest interlayered Cr atoms. Within the slightly distorted octahedral Cr$_6$C, the opposite Cr atoms (180° Cr$_{±}$−C−Cr$_{±}$ groups) account for the antiferromagnetic superexchange since both the Cr 3d orbitals couple to the near-orthogonal C 2p orbitals, resulting in the possibility of an electron on one d-orbital to reach the d-orbital on the other site. In this case, the ferromagnetic superexchange processes start to compete with the antiferromagnetic superexchange mechanism.

The spin density distributions are displayed in Figure 8 to visualize the magnetic ordering of the two Cr atoms in Cr$_2$CO$_2$ and Cr$_2$NO$_2$. The yellow spherical isosurfaces represent the spin-up electrons, while the blue ones are the spin-down electrons. Clearly, the two Cr atoms are parallel in spin-up (yellow), verifying the ferromagnetic ordering in both Cr$_2$CO$_2$ and Cr$_2$NO$_2$.

**CONCLUSIONS**

In summary, the geometrical stabilities and the electronic structure of Cr$_2$CO$_2$ and Cr$_2$NO$_2$ MXene were extensively studied in this work. The energy and phonon spectrum calculations verify the stabilities of the structures, where the functionalized O atoms are located at the top of the C atoms of the Cr$_6$C slab, while situating at the hollow sites of adjacent carbon atoms of the Cr$_2$N slab, respectively. The ferromagnetism of the two MXene materials was predicted by the more accurate HSE method. The band structure calculations manifest that Cr$_2$CO$_2$ is a ferromagnetic semiconductor, while Cr$_2$NO$_2$ possesses a half-metallic feature. The orbital-projected components of the band structures and density of states were thoroughly analyzed to explain the mechanism of ferromagnetism. Our theoretical work might be beneficial to the research on the spintronics of two-dimensional materials.

**COMPUTATIONAL METHODS**

First-principles calculations were performed using the Vienna ab initio simulation package (VASP). The spin-polarized Perdew–Burke–Ernzerhof (PBE) potential of the generalized gradient approximation (GGA) was adopted for the exchange–correlation description. To describe the strong correlation effects in 3d transition metal atoms, the DFT + U approach with $U_{pd} = 4$ eV for Cr was used to optimize the primary structures to find the most stable configuration. The HSE method was used for more accurate structure optimization followed by the band structure calculations, which is known for the notable correction of band gaps. The cut-off energy for plane wave basis is set as 450 eV, large enough for guaranteeing the accuracy of our calculations. The structure relaxation criterion is that the force on each atom is smaller than 0.01eV/Å. The k-point grid was sampled with 15 × 15 × 1 and 7 × 7 × 1 for DFT + U and HSE calculations, respectively. A vacuum region of 30 Å was added above the supercells to avoid the artificial interaction between the vertical images. Furthermore, the phonon dispersion calculations were performed by the PHONOPY code, and the charge and magnetic moment analysis was carried out by the Bader analysis method.

**AUTHOR INFORMATION**

**Corresponding Authors**

Zhiyun Tan — School of Physics and Electronic Science, Zunyi Normal University, Zunyi 563006, Guizhou, China; Email: zytan@zync.edu.cn

Baihai Li — School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 611731, Sichuan, China; orcid.org/0000-0002-9266-1791; Email: libaihai@uestc.edu.cn

**Authors**

Zhenxing Fang — School of Physics and Electronic Science, Zunyi Normal University, Zunyi 563006, Guizhou, China

Youchang Yang — School of Physics and Electronic Science, Zunyi Normal University, Zunyi 563006, Guizhou, China

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.0c03176

**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

This work was supported by the Foundation of Guizhou Science and Technology Department under Grant No. QKHI-LHZ[2017]7091, the Key Disciplines of Physics of Guizhou Province (QXWB[2015]26H), and the National Natural Science Foundation of China (No. 11865019).

**REFERENCES**

1. Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A. Electric Field Effect in Atomically Thin Carbon Films. Science 2004, 306, 666–669.
2. Novoselov, K. S.; Jiang, D.; Schedin, F.; Booth, T. J.; Khotkevich, V. V.; Morozov, S. V.; Geim, A. K. Two-dimensional atomic crystals. Proc. Natl. Acad. Sci. U.S.A. 2005, 102, 10451–10453.
(3) Mak, K. F.; Lee, C.; Hone, J.; Shan, J.; Heinz, T. F. Atomically Thin Si[\text{mathrm{MoS}}]_2: A New Direct-Gap Semiconductor. 
Phys. Rev. Lett. 2010, 105, No. 136805.

(4) Tusche, C.; Meyerheim, H. L.; Kirschner, J. Observation of Depolarized ZnO(001) Monolayers: Formation of Unreconstructed Planar Sheets. 
Phys. Rev. Lett. 2007, 99, No. 026102.

(5) Naguib, M.; Mochalin, V. N.; Barsoum, M. W.;戈格石, Y. 25th Anniversary Article: MXenes: A New Family of Two-Dimensional Materials. 
Adv. Mater. 2014, 26, 992–1005.

(6) Naguib, M.; Kurtoglu, M.; Presser, V.; Lu, J.; Niu, J.; Heon, M.; Hultman, L.;戈格石, Y.; Barsoum, M. W. Two-Dimensional Nanocrystals Produced by Exfoliation of Ti3AlC2. 
Adv. Mater. 2011, 23, 4248–4253.

(7) Naguib, M.; Mashtalir, O.; Carle, J.; Presser, V.; Lu, J.; Hultman, L.;戈格石, Y.; Barsoum, M. W. Two-dimensional transition metal carbides. 
ACS Nano 2012, 6, 1322–1331.

(8) Zha, X.-H.; Luo, K.; Li, Q.; Huang, Q.; He, J.; Wen, X.; Du, S. Role of the surface effect on the structural, electronic and mechanical properties of the carbide MXenes. 
Eurphys. Lett. 2015, 111, No. 26007.

(9) Khazaei, M.; Arai, M.; Sasaki, T.; Estili, M.; Sakka, Y. Two-dimensional molybdenum carbides: potential thermoelectric materials of the MXene family. 
Phys. Chem. Chem. Phys. 2014, 16, 7841–7849.

(10) Wang, K.; Zhou, Y.; Xu, W.; Huang, D.; Wang, Z.; Hong, M. Fabrication and thermal stability of two-dimensional carbide Ti3C2 nanosheets. 
Ceram. Int. 2016, 42, 8419–8424.

(11) Zha, X.-H.; Zhou, J.; Zhou, Y.; Huang, Q.; He, J.; Francisco, J. S.; Luo, K.; Du, S. Promising electron mobility and high thermal conductivity in Sc2CNT2 (T = F, OH) MXenes. 
Nanoscale 2016, 8, 6110–6117.

(12) Naguib, M.; Come, J.; Daytakin, B.; Presser, V.; Taberena, P.-L.; Simon, P.; Barsoum, M. W.;戈格石, Y. MXene: a promising transition metal carbide anode for lithium-ion batteries. 
Electrochem. Commun. 2012, 16, 61–64.

(13) Yoon, Y.; Lee, K.; Lee, H. Low-dimensional carbon and MXene-based electrochemical capacitor electrodes. 
Nanotechnology 2016, 27, No. 172001.

(14) Lukatskaya, M. R.; Mashtalir, O.; Ren, C. E.; Dall’Agnese, Y.; Rozier, P.; Taberena, P. L.; Naguib, M.; Simon, P.; Barsoum, M. W.;戈格石, Y. Cation Intercalation and High Volumetric Capacitance of Two-Dimensional Titanium Carbide. 
Science 2013, 341, 1502–1505.

(15) Xu, B.; Zha, X.; Zhang, W.; Zhen, X.; Pei, Z.; Xue, Q.; Zhi, C.; Shi, P. Ultrathin MXene-Micropattern-Based Field-Effect Transistor for Probing Neural Activity. 
Adv. Mater. 2016, 28, 3333–3339.

(16) Dong, L.; Kumar, H.; Anasori, B.;戈格石, Y.; Shenoy, V. B. Rational Design of Two-Dimensional Metallic and Semiconducting Spintron Materials Based on Ordered Double-Transition-Metal MXenes. 
J. Phys. Chem. Lett. 2017, 8, 422–428.

(17) Kumar, H.; Frey, N. C.; Dong, L.; Anasori, B.;戈格石, Y.; Shenoy, V. B. Tunable Magnetism and Transport Properties in Nitride MXenes. 
ACS Nano 2017, 11, 7648–7655.

(18) Choudhuri, I.; Bhauriyal, P.; Pathak, B. Recent Advances in Graphene-like 2D Materials for Spintronics Applications. 
Chem. Mater. 2019, 31, 8260–8285.

(19) Kim, H.; Alshareef, H. N. MXetronics: MXene-Enabled Electronic and Photonic Devices. 
ACS Mater. Lett. 2020, 2, 55–70.

(20) Khazaei, M.; Arai, M.; Sasaki, T.; Chung, C.-Y.; Venkataramanan, N. S.; Estili, M.; Sakka, Y.; Kawazoe, Y. Novel Electronic and Magnetic Properties of Two-Dimensional Transition Metal Carbides and Nitrides. 
Adv. Funct. Mater. 2013, 23, 2185–2192.

(21) Si, C.; Zhou, J.; Sun, Z. Half-Metallic Ferromagnetism and Surface Functionalization-Induced Metal-Insulator Transition in Graphene-like Two-Dimensional Cr2C Crystals. 
ACS Appl. Mater. Interfaces 2015, 7, 17510–5.

(22) Heyd, J.; Scuseria, G. E.; Ernzerhof, M. Hybrid functionals based on a screened Coulomb potential. 
J. Chem. Phys. 2003, 118, 8207.