Conversation from anti-ferromagnetic MnBr2 to ferromagnetic Mn3Br8 monolayer with large MAE

Yan Hu
Northwestern Polytechnical University

Shuo Jin
Northwestern Polytechnical University

Zhifen Luo
Northwestern Polytechnical University

Hanghang Zeng
Northwestern Polytechnical University

Jiahui Wang
Northwestern Polytechnical University

Xiao-Li Fan (✉️ xlfan@nwpu.edu.cn)
Northwestern Polytechnical University  https://orcid.org/0000-0002-5291-0706

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Dear Editor:

We would like to submit the enclosed manuscript entitled “Conversation from anti-ferromagnetic MnBr$_2$ to ferromagnetic Mn$_3$Br$_8$ monolayer with large MAE”, which we wish to be considered for publication in the Nanoscale Research Letters. This manuscript is approved by all authors for publication. We would like to declare that the work described is original research that has not been published previously, and not under consideration for publication elsewhere, in whole or in part.

2D magnets with Curie temperature higher than liquid-nitrogen temperature (77K), large magnetic moment, and large magnetic anisotropy energy (MAE) are highly desirable in spintronics. We design Mn$_3$Br$_8$ monolayer via inducing Mn vacancy at 1/4 population in MnBr$_2$ monolayer which is antiferromagnetic with large magnetic moment of 5$\mu_B$ for each Mn atom. Such defective configuration is designed to change the coordination structure of the Mn-d$^5$, to achieve ferromagnetism with large magnetic moment and large MAE. Our calculations show that Mn$_3$Br$_8$ monolayer is a FM half-metal and has Curie temperature higher than 77K, large MAE of -2.33meV per formula unit. Plus, each Mn atom has large atomic magnetic moment of 13/3$\mu_B$. Additionally, Mn$_3$Br$_8$ monolayer maintains to be FM under small biaxial strain. Both biaxial strain and carrier doping make the MAE increase. Our designed defective structure of MnBr$_2$ monolayer provides a simple but effective way to achieve ferromagnetism with large MAE and large magnetic moment.

We believe our paper may be particularly interest to the readers of Nanoscale Research Letters.

Thank you very much for your consideration.

Yours sincerely,

Xiaoli Fan

School of Materials Science and Engineering, Northwestern Polytechnical University
Conversation from anti-ferromagnetic MnBr\textsubscript{2} to ferromagnetic Mn\textsubscript{3}Br\textsubscript{8} monolayer with large MAE

Y. Hu, \textsuperscript{1} S. Jin, \textsuperscript{2} Z. F. Luo, \textsuperscript{1} H. H. Zeng, \textsuperscript{1} J. H. Wang \textsuperscript{1}, X.L. Fan \textsuperscript{1*}

\textsuperscript{1} State Key Laboratory of Solidification Processing, Center for advanced lubrication and seal Materials, School of Material Science and Engineering, Northwestern Polytechnical University, 127 YouYi Western Road, Xi’an, Shaanxi 710072, China

\textsuperscript{2} Queen Mary University of London Engineering School, Northwestern Polytechnical University, 127 YouYi Western Road, Xi’an, Shaanxi 710072, China

Abstract

A pressing need in low energy spintronics is two-dimensional (2D) ferromagnets with Curie temperature above the liquid-Nitrogen temperature (77K), sizeable magnetic anisotropy. We studied Mn\textsubscript{3}Br\textsubscript{8} monolayer which is obtained via inducing Mn vacancy at 1/4 population in MnBr\textsubscript{2} monolayer. Such defective configuration is designed to change the coordination structure of the Mn-d\textsuperscript{5}, to achieve ferromagnetism with sizeable magnetic anisotropy energy (MAE). Our calculations show that Mn\textsubscript{3}Br\textsubscript{8} monolayer is a ferromagnetic (FM) half-metal and has Curie temperature of 130K, large MAE of -2.33meV per formula unit, atomic magnetic moment of 13/3μ\textsubscript{B}. Additionally, Mn\textsubscript{3}Br\textsubscript{8} monolayer maintains to be FM under small biaxial strain, whose Curie temperature under 5% compressive strain is 160K. Additionally, both biaxial strain and carrier doping make the MAE increase, which mainly contributed by the magneto-crystalline anisotropy energy (MCE). Our designed defective structure of MnBr\textsubscript{2} monolayer provides a simple but effective way to achieve ferromagnetism with large MAE in 2D materials.

1. Introduction

Spintronics exploiting the electron spin and the associated magnetic moment, has attracted extensive attention during the past few decades \cite{1}, because of its unique advantages over charge-based devices. Recently, the discovery of two-dimensional (2D) ferromagnents with long-range magnetic ordering at finite temperature \cite{2,3} are of great significance for nanoscale spintronics and related applications, which inspires tremendous efforts in investigations and fabrications of 2D ferromagnets \cite{4-9}.
The first two 2D FM materials with atomic-thickness was achieved in 2017, that are monolayer CrI$_3$ [2] and bilayer Cr$_2$Ge$_2$Te$_6$ [3]. Unfortunately, both their Curie temperature are lower than the liquid-nitrogen temperature (77K), which limits their realistic applications. Besides the Curie temperature, sizeable magnetic anisotropy and magnetic moment are also indispensable for practical application. Large magnetic anisotropy energy (MAE) implies the benefit for the magnetic ordering against the heat fluctuation, and the possibility to reduce the grain size per bit of information; small MAE may result in super-paramagnetic rather than ferromagnetic. Large magnetic moment provides higher sensitivity, higher efficiency, and higher density for spintronics. Heavy elements are more likely to bring in large MAE due to their strong SOC effect [10]. A series of 2D FM materials composed of heavy elements have been predicted having large MAE, such as CrI$_3$ [11], CrAs [12], CrSeI [13], CrSiTe$_3$ [14], CrW$_6$ [15], FeBr$_2$ and FeI$_2$ monolayers [16]. Additionally, the local magnetic moment on Mn atom of MXenes Mn$_2$NF$_2$ and Mn$_2$N(OH)$_2$ is 4.5μB per Mn atom [17], which is the largest reported for FM 2D materials.

Since CrI$_3$ monolayer has been synthesized, transition-metal halides have attracted much attentions [18-27]. Particularly, spin Seeback effect has been observed in bilayer MnF$_2$ [20]; few layers of CrI$_3$ has been implemented into the magnetic tunneling junctions (MTJ), demonstrating ultrahigh magnetoresistance even up to 1000000% [21]; NiCl$_3$ monolayer has been predicted to be a novel Dirac spin-gapless semiconductor (SGS) [22]. Particularly, MnBr$_2$ monolayer is antiferromagnetic with 0.25meV MAE along the perpendicular direction to the plane [16] based on the first-principles calculations; Mn$^{2+}$ ions are in the d$^5$ high-spin state with magnetic moment of 5μB [16, 26]. These results imply the potential of MnBr$_2$ as monolayer ferromagnet with large magnetic moment. The key problem is how to convert the AFM coupling Mn ions into FM coupling.

Significant density of Mn vacancy was observed experimentally in LaMnO$_3$ thin films [28], and the concentration of defects can be controlled by regulating the synthesis process deliberately via irradiation of high energy particles, or chemical etching [29]. In this context, we designed the Mn$_3$Br$_8$ monolayer by inducing single Mn vacancy to MnBr$_2$ monolayers. Mn vacancy will change the coordination structure of the Mn atom, and break the d$^5$ configuration, which may convert the anti-ferromagnetic coupling into ferromagnetic coupling and bring in large MAE due to the heavy Br atom. As we expect, Mn$_3$Br$_8$ monolayer is FM and has large MAE of -2.33 meV per formula unit, the magnetic moment for each Mn atom is 13/3μB. Considering the easy introducing of strain via bending flexible substrates [30-33], elongating elastic substrate [33-35], exploiting the thermal expansion mismatch [33,36], and so on [33], and the effective control on the spin polarization of
2D materials via electrostatic doping [37,38], we also studied the Mn3Br8 monolayer under biaxial strain and carrier doping. Our results show that Mn3Br8 monolayer maintains to be FM with Curie temperature increasing under small biaxial strain. Plus, both biaxial strain and carrier doping make the MAE increase.

2. Computational methods

All the calculations in the present study were performed by adopting the spin-polarized density function theory (DFT) method as implemented in the Vienna ab-initio simulation package (VASP) [39]. Interactions between electrons and nuclei were described by the projector augmented wave (PAW) method [40,41], and the electronic exchange-correlation interactions were described by the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) method [42]. The Hubbard U terms were adopted to calculate the strong-correlated interaction [43]; an effective on-site coulomb interaction parameter (U) of 4eV and an exchange energy (J) of 1eV which was adopted for studying Mn-incorporated 2D materials were used for the Mn-d electrons [44]. The Brillouin zone integration was carried out by 9×9×1 k-mesh based on the Monkhorst-Pack scheme [45]. The phonon spectrums were calculated using the Phonopy code [46] which is implemented within the VASP package. A vacuum space of 20Å was added along the direction perpendicular to the surface of the monolayer to avoid the interaction between the adjacent layers. The cutoff energy for the plane wave basis set was set as 500eV. The convergence criterion for the total energy and force were set as 1×10^{-6} eV and 0.01 eV/Å, respectively.

3. Results and discussions

3.1 Cleavage energy, ground state, and stability of the MnBr2 monolayer

The optimized lattice constants of bulk MnBr2 are a=b=3.95Å, consistent with the previous experimental result (a=b=3.87Å) [25]. We firstly explored the feasibility of exfoliating MnBr2 monolayer from the bulk MnBr2. Fig. 1(a) presents the well-known, effective, and widely approved method of calculating the cleavage energy [47-49]. Specifically, the cleavage energy was obtained by calculating the variation of the total energy with respect to the separation $d$ between the facture parts as shown in Fig. 1(a). The interlayer long-range vdW interactions was described by the Grimme’s DFT-D2 scheme [50,51]. The total energy increases with $d$, and then slowly converges as showing in Fig. 1(b). The calculated cleavage energy is 0.10 J/m², which is smaller compared with graphene (0.35 J/m²) [52], demonstrating the feasibility of obtaining MnBr2 monolayer via micro-mechanical exfoliating method.
MnBr$_2$ monolayer has the $C_{3v}$ symmetry as showing in Fig. 1(c); each Mn atom is surrounded by 6 neighboring Br atoms, forming an octahedral [MnBr$_6$]$^{4-}$ unit. As showing in Fig. S1(a) and (b), three possible magnetic configurations, namely non-magnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM) states are considered. Our results show that the ground state of MnBr$_2$ monolayer is the AFM state, which is more stable than the NM and FM states by 3.91 eV and 0.9meV per formula unit, respectively. The MAE is 0.25meV, the positive value indicating that the easy magnetization axis is along the out-of-plane directions, agreeing with previous result [16]. The optimized lattice constants are $a=b=3.95\text{Å}$, same with the lattice constants of the bulk MnBr$_2$. The Mn-Br bond length is 2.73Å, and the vertical distance between the two halide planes is 3.03Å.

The stability of the MnBr$_2$ monolayer was further investigated by calculated the formation energy, phonon spectrum, and elastic constants. The formation energy is calculated as:

$$E_{\text{form}} = E_{\text{MnBr}_2} - E_{\text{Mn}} - 2E_{\text{Br}}$$

where $E_{\text{MnBr}_2}$ represents the energy of MnBr$_2$ monolayer, $E_{\text{Mn}}$ and $E_{\text{Br}}$ are the energies of Mn and Br atoms in their bulk structures, respectively. The calculated $E_{\text{form}}$ is -1.87eV per atom; the negative value means that the formation is exothermic and MnBr$_2$ monolayer is energetically favorable. Plus, our calculated phonon spectrum (Fig. 1(d)) for MnBr$_2$ monolayer shows no negative frequency in the whole Brillouin zone, indicating dynamically stable. Additionally, the calculated elastic constants (Table S1) comply with the Born-Huang criteria [53] of $C_{11} > 0$, $C_{11}C_{22} - C_{12}^2 > 0$ and $C_{66} > 0$, confirming that MnBr$_2$ monolayer is mechanically stable. The $C_{11}$ and $C_{22}$ are equal to each other, which exhibits the mechanical isotropy; the rigidity against deformation are about three times softer along the c direction comparing with that along the a or b directions. The calculated in-plane stiffness is 26.98 J/m$^2$, about 75% of the MnPSe$_3$ (36 J/m$^2$) [49], and 15% of MoS$_2$ monolayer (180 J/m$^2$) [54]. Plus, MnBr$_2$ monolayer demonstrates higher flexibility, and the ability of sustaining larger tensile strain comparing with MoS$_2$ monolayer (11%) [54]. This may attribute to ionic bonds for MnBr$_2$ monolayer against the covalent bonds of MoS$_2$ monolayer.

Additionally, the gravity induced out-of-plane deformation is estimated by the following equation via using the in-plane stiffness [55]:

$$c_{\text{def}} = \frac{F}{E_{\text{in-plane}}A}$$

where $F$ is the applied force, $E_{\text{in-plane}}$ is the in-plane stiffness, and $A$ is the area of the monolayer.
where $\rho = 4.91 \times 10^{-4} \text{Kg/m}^2$ is the mass density of MnBr$_2$, and $L$ is the size of the monolayer. Taking $L \approx 100 \mu\text{m}$, we obtain $\frac{h}{L} \approx 5.72 \times 10^{-4}$, which is comparable to that of monolayer CrI$_3$ ($6.45 \times 10^{-4}$) [47], and is of the same magnitude order of graphene [55]. Our result shows that the free-standing MnBr$_2$ monolayer can withstand its own weight and maintain the planar structure.

The electronic band structure of MnBr$_2$ monolayer is shown in Fig. 1(e), which indicates that MnBr$_2$ monolayer is AFM semiconductor with a direct band gap of 3.35eV. Both valence band maximum (VBM) and conduction band minimum (CBM) locate at the $\Gamma$ point. To gain insight of the electronic structures, projected density of states (DOS) for the Mn-d and Br-p orbital are presented in Fig. 1(f). The five d orbitals of Mn$^{2+}$ ion split into $a(d_{x^2})$, $e_g(d_{xy} + d_{yz})$, and $e_g(d_{xy} + d_{x^2-y^2})$ groups according to the $C_{3v}$ symmetry, and the five d-electrons occupy the five spin-up channels of the d-orbitals. Correspondingly, Mn$^{2+}$ ion is in the d$^5$ high-spin state with the magnetic moment of 5$\mu_B$. Meanwhile, the Br$^{1-}$ ion is in the 4p$^6$ low-spin state with neglectable magnetic moment (Fig. S2(a)). According to the Goodenough-Karamori-Anderson (GKA) rule, such configuration always demonstrates antiferromagnetic coupling [56].

3.2 Stability, electronic and magnetic properties of Mn$_3$Br$_8$ monolayer

Mn vacancy was introduced to break the d$^5$ configuration of the Mn$^{2+}$ ions. Single Mn vacancy is introduced in the $2 \times 2 \times 1$ supercell of MnBr$_2$ monolayer, which gives out the Mn$_3$Br$_8$ monolayer. As showing in Fig. 2(a), each Mn atom has four nearest neighboring Mn atoms and binds to six Br atoms, forming a distorted octahedral [MnBr$_6$] unit. Five magnetic states (NM, FM, FIM, AFM-1, and AFM-2) shown in Fig. S3 were considered. Our results indicate that the FM state is the ground state, which is more stable than the other four by 9.84eV, 32.90 meV, 129.85 meV, and 97.65meV per formula unit, respectively. The optimized lattice constant is still 3.95Å. Different from MnBr$_2$ monolayer, Mn$_3$Br$_8$ monolayer has 2 types of Mn-Br bonds (Fig. 2(b)). The bonds between Mn atom and the two central Br atoms ($d_{\text{Mn-Br1,2}}$) are 2.76Å, while the other Mn-Br bonds ($d_{\text{Mn-Br3,4,5,6}}$) are 2.59Å. The vertical distance between the two halide planes is 3.33Å.

To verify the feasibility of inducing single Mn vacancy, we firstly calculated the vacancy
formation energies under different experimental conditions (See details on Page 1 of SI). As showing in Fig. 2(c), the formation energies under Mn-rich/Br-rich environment is 6.30/0.71 eV per Mn vacancy, indicating that the formation of Mn vacancy is energetically more favorable under the Br-rich environment. Indeed, the S vacancy has been experimentally achieved in MoS$_2$ monolayer [57], and the predicted formation energy of S vacancy in MoS$_2$ monolayer under the S-rich environment is 2.35eV [58]. In this context, Mn$_3$Br$_8$ monolayer is synthetically approachable. Plus, there is no negative frequency found in its phonon spectrum shown in Fig. 3(a), proving the dynamically stable. These results approve our design of introducing Mn vacancy to bring in ferromagnetism.

The ferromagnetism of Mn$_3$Br$_8$ monolayer attributes to the FM super-exchange interaction. According to the Goodenough-Kanamori-Anderson (GKA) rule [56], the super-exchange between the Mn ions is FM when the Mn-Br-Mn angle is close to 90°. In such configuration (Fig. S4), the Mn-d orbital tend to AFM couples with different orthogonal Br-p orbital, thus the indirect Mn-Mn magnetic coupling is expected to be FM. But if each Mn ion has 5 unpaired electrons, it will be AFM coupling, which is true for MnBr$_2$ monolayer. There are existing two different super-exchange interaction paths in Mn$_3$Br$_8$ (Fig. 2(a)), and both are FM. One involves central Br1,2 atoms with Mn-Br bond lengths of 2.76Å and Mn-Br-Mn angles of 87.5°; the other one involves Br3,4,5,6 atoms with Mn-Br bond length of 2.59Å and Mn-Br-Mn angles of 95°. Particularly, hybridized interactions between p orbitals of Br3,4,5,6 atoms and Mn-d orbitals are stronger than that of p-d hybridization involving Br1,2 atoms, as showing in Fig. 3(c), specially from -2eV to -1.4eV. While from -1.4eV to -0.9eV, p-d hybridization involving Br1,2 atoms are dominated.

The valence electrons of Br$^{+}$ ion (4p$^6$) fully occupy both spin-up and spin-down channels as showing in Fig. 3(c), correspondingly, the atomic magnetic moments of Br atoms are neglectable (Fig. S2(b)). Meanwhile, the Mn ions having 13/3 d electrons are in the high spin-state with 13/3μB atomic magnetic moment. For each Mn ion, 2/3 d-orbital is unoccupied; the spin-up channel of both $e_1$ and $e_2$ orbitals are partially occupied and crossing the Fermi level, resulting in half-metallicity. The half-metallic character also can be observed from the spin-resolved electronic band structure shown in Fig. 3(b). The spin-up channel is metallic, while the spin-down channel is semiconducting with the indirect band gap of 2.97eV; the VBM/CBM locates at the $M$ / $\Gamma$ point. The value of the band gap is close to those of the MnP (2.86eV) [59], MnAs (2.92eV) [59], Ni$_2$NO$_2$ (2.98eV) [60], and large enough to prevent the thermally excited spin-flip.
The magnetic orientations are determined by the magnetic anisotropy energy (MAE). The MAE of magnetic solids arises from two contributors, namely, the magneto-crystalline energy (MCE) related to the spin-orbit coupling (SOC), and the magnetic dipolar anisotropy energy (MDE) attributed by the magneto-static dipole-dipole interaction. The MDE in the 3D isotropic materials, such as bcc Fe and fcc Ni, is very small. But for low-dimensional materials composed of transition metal atoms with large magnetic moment, the MDE is not neglectable [61-63]. The MCE is defined as the difference between the magnetization energy along the in-plane (100 or 010) and out-of-plane (001) directions by taking the SOC into account. The MDE is obtained as the difference of \( E_d \) between the in-plane and out-of-plane magnetizations. \( E_d \) in atomic Rydberg units is given by [61,62]

\[
E_d = \sum_y \frac{2m_i m_j}{c^2} M_{ij}
\]

where the speed of light, \( c = 274.072 \), \( i/j \) are the atomic position vectors in the unit cell, and \( m_i/m_j \) is the atomic magnetic moment (\( \mu_B \)) on site \( i/j \). The magnetic dipolar Madelung constant \( M_{ij} \) is calculated via

\[
M_{ij} = \sum_R \left\{ \frac{1}{|R+i+j|^3} \left[ 1 - 3 \left( \frac{(R+i+j) \cdot m_i}{|R+i+j|^2} \right)^2 \right] \right\}
\]

where \( R \) are the lattice vectors. In a 2D material, since all the \( R \) and \( i \) are in-plane, the second term would be zero for the out-of-plane magnetization, resulting in the positive \( M_{ij} \), while \( M_{ij} \) is negative for an in-plane magnetization [63]. Therefore, the MDE relates to the magnetic moment of transition metal, and always prefers the in-plane magnetization.

The calculated MCE for Mn\(_3\)Br\(_8\) monolayer is -1.90meV per formula unit (Fig. 4(a)), much larger than those of bulk Fe (0.001meV per atom), and Ni (0.003meV per atom) [64], and larger than that of the Fe monolayer on Rh (111) (0.08meV per atom) [65], suggesting the thermal stability of the magnetization of the Mn\(_3\)Br\(_8\) monolayer. The relationship between the MCE and the azimuthal angle can be described by the following equation [66]:

\[
MCE(\theta) = A \cos^2(\theta) + B \cos^4(\theta)
\]
where $A$ and $B$ are the anisotropy constants and $\theta$ is the azimuthal angle. The fitting result is shown in Figs. S5. Additionally, the evolution of MCE as the spin axis rotates through the whole space is illustrated in Fig. 4(b). MCE within the xy plane show no difference, but reaches the maximum value along the direction perpendicular to the xy plane, confirming the strong magnetic anisotropy. The MDE is -0.43meV per formula unit, and MAE (MCE+MDE) is -2.33meV per formula unit. The negative value indicates that the easy magnetization axis is along the in-plane directions. The MDE does not change the magnetic orientation, but enhance the MAE and the magnetization. Additionally, the MAE of Mn$_3$Br$_8$ monolayer is much larger than that of MnBr$_2$ monolayer, proving again the effectiveness of our design.

We further calculated the $T_c$ for FM Mn$_3$Br$_8$ monolayer by performing the Monte Carlo (MC) simulations based on the Heisenberg model, which has been proven to be the effective method for predicting $T_c$ for 2D materials [11,15,48,59,67-72]. Our estimated $T_c$ of CrI$_3$ monolayer is 42K [72], agreeing well with the experimental measured value [2] and previous calculation results [15,59,67,68,70,72], which proves the accuracy of our adopted method. The spin-Hamiltonian including the nearest neighboring (NN) magnetic interaction is described as

$$H = - \sum_{i,j} J_{M,i} M_j$$

where $J$ is the NN magnetic exchange parameter, $M_{i,j}$ is the net magnetic moment of Mn ions, $i$ and $j$ stand for the NN pair of Mn ions. The magnetic coupling parameter $J$ is calculated via the energy difference between the FM and AFM states as

$$J = \frac{E_{AFM} - E_{FM}}{16M^2}$$

The calculated $J$ of NN Mn ions is 1.01meV; the positive value indicates the preferring of FM coupling.

The calculated $J$ of the NN Mn ions and the 100×100×1 supercell containing 20000 magnetic moment vectors was adopted to perform the MC simulations. The simulations at each temperature lasts for $10^5$ steps. Each magnetic moment vector rotates randomly in all directions. Fig. 3(d) shows the evolution of specific heat defined as $C_v = \langle (E^2) - \langle E \rangle^2 \rangle / R T^2$ with temperature, from which we obtained the $T_c$ of 130 K for Mn$_3$Br$_8$ monolayer by locating the peak position of $C_v$, higher
than the liquid-nitrogen temperature (77 K), and $T_c$ of CrI$_3$ (45K) [2] and Cr$_2$Ge$_2$Te$_6$ (28K) [3], CrX$_3$ (X=F, Cl, Br) (36~51K) [11], CrXTe$_3$ (X=Si, Ge) (35.7K, 57.2K) [48]. Our calculations demonstrate that the FM Mn$_3$Br$_8$ monolayer has the large MAE and Curie temperature higher than the liquid-nitrogen temperature.

3.3 Mn$_3$Br$_8$ monolayer under biaxial strain and carrier doping

Strain engineering has been proven applicable for many 2D materials, and effective to alter the structural parameters, such as the bond lengths and angles, and to tune the electronic and magnetic properties. In this context, we investigated Mn$_3$Br$_8$ monolayer under the biaxial strain ranging from -5% to 5%. It turns out that Mn$_3$Br$_8$ monolayer under biaxial strain from -5% to 5% maintains to be FM and the atomic magnetic moment hardly changes. As showing in Figs. 5(a) and (c), the angles between two Mn atoms and Br1,2 atoms ($\theta_{\text{Mn-Br1,2-Mn}}$) are 84°-90°, which increases as the strain and gradually approaches 90°. The Mn-Br-Mn angles involving Br3,4,5,6 atoms ($\theta_{\text{Mn-Br3,4,5,6-Mn}}$) gradually deviate from 90°, ranging from 90° to 100°. Thus, super-exchange interactions between the Mn ions mediated via different orthogonal Br-p orbital are still FM.

The Mn-Mn and Mn-Br distances all increase monotonically as the strain changing from -5% to 5%. Correspondingly, the exchange parameter under the biaxial strain presented in Fig. 6(a) decreases with the biaxial strain changing from -5% to 5% and reach the largest value (1.18meV) under -5% biaxial strain. The Curie temperature of Mn$_3$Br$_8$ monolayer under -5% biaxial strain is 160 K (Fig. 7(a)). Particularly, the Mn-Br bonds under the increasing tensile strain become longer, and the angles of Mn-Br3,4,5,6-Mn deviate from 90°, which are the main reason why the FM super-exchange interaction become weaker. Consequently, the Curie temperature decreases. It is similar with CrPTe$_3$ and FePS$_3$ monolayers [73]. Additionally, the MDE decreases with the increasing strain (Fig. S7(b)); the MAE under -1% biaxial strain is the largest (-3.04meV). The -5%~5% strain does not cause large structural deformation for Mn$_3$Br$_8$ monolayer, and the morphology of its band structures hardly changes. Mn$_3$Br$_8$ monolayer keeps to be half-metallic. Both VBM and CBM in the semiconducting spin-channel move upwards slightly to the higher energy as shown in Fig. 6(c) and Figs.8; the band gap increases slowly with the increasing biaxial strain to 3.12eV under 5% biaxial strain.

Electron/hole doping always leads to VBM/CBM moving away from the Fermi level. Our calculations show that Mn$_3$Br$_8$ monolayer with -1~1e ($\sim 1.7 \times 10^{14} \text{cm}^{-2}$) carrier doping per formula
unit is still FM; the atomic magnetic moment of each Mn ion is still 13/3μB. As showing in Figs. 5(b) and (d), with carrier doping from -1e to 1e per formula unit, the Mn-Br-Mn angles involving Br3,4,5,6 atoms are about 90° ~ 98°; the Mn-Br1,2-Mn angles are about 88° ~ 90°. The Mn-Mn and Mn-Br1,2 distances increase with the increasing electron doping. Mn3Br8 monolayer with 0.2e and 0.4e carrier doping has larger magnetic exchange parameter (Fig. 6(a)). The Curie temperature at 0.2e electron doping is largest of 140K (Fig. 7(b)). Additionally, with -1e~0.2e doping, the MAE is along in-plane directions; the MDE decreases with the increasing electron doping. Under 0.4e doping, the MCE turns to be positive with the value of 0.41meV per formula unit; the MAE is only 0.01meV per formula unit with taking the MDE into account (Fig. S7(a) and (b)). With 0.6e, 0.8e and 1e doping, the PMA (perpendicular magnetic anisotropy energy) is 1.70, 2.42, and 5.13 meV, respectively, large enough for spintronic applications (Fig. 6(b)).

Additionally, Mn3Br8 monolayer with carrier doping -1e ~ 1e per formula unit maintains to be half-metal. Its band gap in the semiconducting spin-channel increases/decreases slightly with the increasing electron/hole doping as showing in Fig. 6(d); the positions of the VBM and CBM do not change. Exceptional, Mn3Br8 monolayer turns to be FM spin-gapless semiconductors (SGS) with the metallic spin-channel opening up a very small energy gap (0.07eV) under -0.6e and -0.8e hole doping; its Fermi level locates in the band gap region (Figs. 9(b) and (c)). Correspondingly, electrons may be easily excited from the valence band to the conduction band with a small input of energy, which simultaneously produces 100% spin polarized electron and hole carriers. The Curie temperature at -0.6e and -0.8e hole doping is 110K (Fig. 7(c) and (d)), higher than liquid-Nitrogen temperature (77K). The charge density modulation of $10^{13} \sim 10^{15} \text{cm}^{-2}$ was already achieved experimentally [74-76], in this context, our predicted properties of Mn3Br8 monolayer with carrier doping is also experimentally approachable.

Conclusions

In summary, the stability, electronic and magnetic properties of Mn3Br8 monolayer have been carefully investigated. Our results show that Mn3Br8 monolayer is FM half-metal with 130K Curie temperature and with 2.97eV band gap for the semiconducting spin-channel. Plus, the magnetic moment of each Mn ion is 13/3μB; the MAE is -2.33meV per formula unit. The Mn3Br8 monolayer is designed by inducing single Mn vacancy in the $2 \times 2 \times 1$ supercell of MnBr2 monolayer to break the AFM coupling d$^5$ configuration. The feasibility of forming the Mn vacancy and the dynamical, mechanical stability of Mn3Br8 monolayer have been comprehensively confirmed. Additionally,
Mn$_3$Br$_8$ monolayer under biaxial strain -5% ~ 5% is still FM half-metal with 2.71~3.12eV band gap for the semiconducting spin-channel, whose Curie temperature under -5% biaxial strain is 160K. Both biaxial strain and carrier doping make the MAE increase, which turns to be perpendicular to the plane under electron doping. With 0.8e and 0.6e hole doping, Mn$_3$Br$_8$ monolayer turns to be spin-gapless semiconductor (SGS) with band gap of 0.07eV. Our calculations demonstrate Mn$_3$Br$_8$ monolayer as FM half-metal with high Curie temperature, and having large MAE and large magnetic moment, and tunable electronic and magnetic properties via applying biaxial strain and carrier doping.

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Compliance with ethical standards

Conflict of interest: the authors declare that they have no conflict of interest.

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(a) Bulk model of MnBr2 used to calculate the cleavage energy, and (b) the cleavage energy as a function of the separation between two fractured parts. (c) Top and side views, (d) phonon spectrum, (e) electronic band structure and (f) projected density of states (PDOS) of Mn-d orbitals and Br-p orbitals for MnBr2 monolayer. represents the vertical distance between two halide planes. The primitive cell is circulated in black dash lines. The Fermi level for band structure and DOS is set as 0eV.
Figure 2

(a) Top and side views for Mn3Br8 monolayer, represents the vertical distance between two halide planes. The primitive cell is circulated in black dash lines; the green arrow lines show two different paths of the super-exchange interaction. (b) Structure of the distorted MnBr6 octahedron. (c) Formation energies for single Mn vacancy as a function of chemical potential of Mn ($\mu_{\text{Mn}}$).
Figure 3

(a) Phonon spectrums, (b) spin-resolved electronic band structure, and (c) projected density of states (PDOS) of Mn-d orbitals and Br-p orbitals for Mn3Br8 monolayer. (d) On-site magnetic moments of Mn atoms and the specific heat as function of temperature based on Heisenberg model for Mn3Br8 monolayer. The Fermi level for band structure and PDOS is set as 0 eV.
The variation of magneto-crystalline anisotropy energy (MCE) (a) with respect to azimuthal angle and (b) in the space for Mn3Br8 monolayer.
Figure 5

The variations of angles between two Mn and Br atoms, the distance between Mn and Br atoms, and distance between nearest neighboring Mn atoms with respect to the applied biaxial strain and carrier doping. Variation of (a) angle and (c) distance with respect to biaxial strain, variations of (b) angle and (d) distance with respect to carrier doping. Positive and negative values of carrier doping represent the electron and hole doping, respectively.

Figure 6

The variations of (a) the exchange parameter and (b) magnetic anisotropy energy (MAE) for Mn3Br8 monolayer with respect to the applied biaxial strain and carrier doping. The variations of valence band maximum (VBM), conduction band minimum (CBM) and band gap in the semiconducting channel for
Mn3Br8 monolayer with respect to (c) the applied biaxial strain and (d) carrier doping ranging. Positive and negative values of the carrier doping represent the electron and hole doping, respectively.

Figure 7

On-site magnetic moments of Mn atoms and the specific heat as function of temperature based on Heisenberg model for Mn3Br8 monolayer (a) under -5% biaxial strain, with (b) 0.2e, (c) -0.6e, and (d) -0.8e carrier doping per formula unit. Positive and negative values represent the electron and hole doping, respectively.
Figure 8

(a)–(j) Spin-resolved band structure for Mn3Br8 monolayer under biaxial strain from -5% to 5%.
Figure 9

(a)~(j) Spin-resolved band structure for Mn3Br8 monolayer with carrier doping from -1e to 1e per formula unit. Positive and negative values represent the electron and hole doping, respectively.

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