Supplementary Information

Discovery of intrinsic two-dimensional antiferromagnets from transition-metal borides

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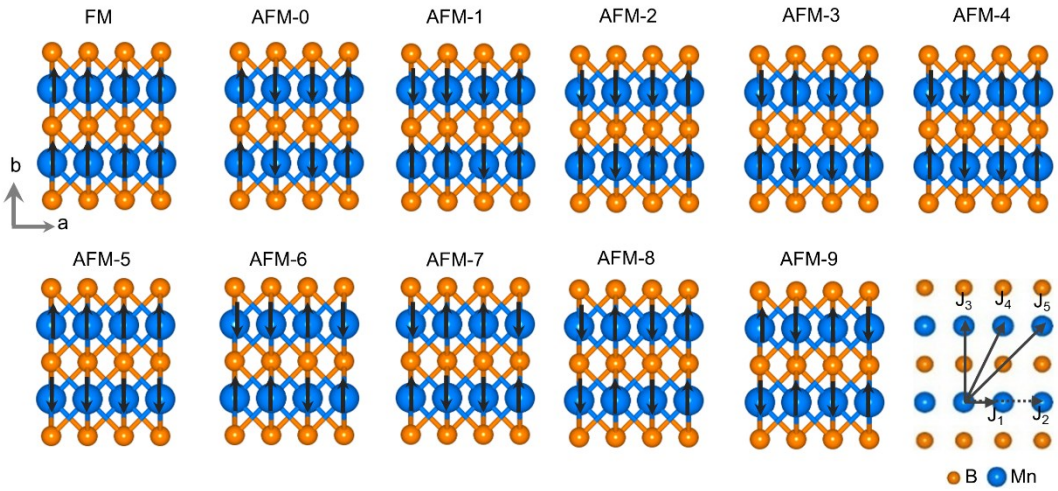


Fig. S1 Top view of eleven collinear magnetic configurations of a 2-D monolayer MBs. FM and AFM-i (i= 0, 1, 2, 3, 4, 5, 6, 7, 8, 9) respectively means ferromagnetic and antiferromagnetic state. J_1, J_2, J_3, J_4, and J_5 are nearest- (1^{st}), second-nearest- (2^{nd}), third-nearest- (3^{rd}), fourth-nearest- (4^{th}), and fifth-nearest-neighbor (5^{th}) magnetic coupling parameters, respectively. The up-arrow and down-arrow respectively represent the spin-up and spin-down state.

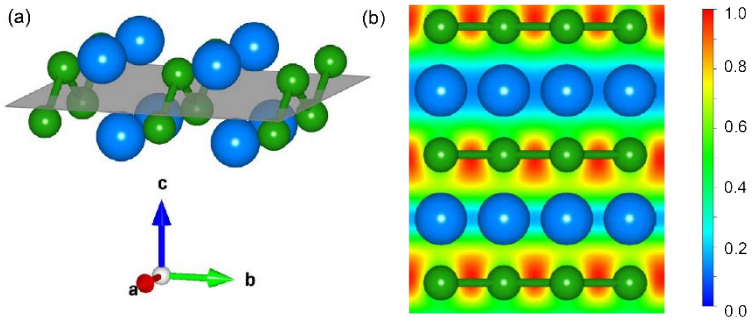


Fig. S2 (a) the plane along (001) direction. (b) calculated electron localization function ELF of 2-D MnB on (001) plane. The isosurface is set to 0.65 e/Å^3. The blue and green balls are respectively Mn and B atoms.

The topological analysis of electron localization function ELF is a very useful tool

for the determination of chemical bonding type.[S1] The values of ELF vary between 0 and 1, in which 1 represents the completely localized character of electrons, while 0 stands for the delocalization of electrons. ELF = 0.5 is corresponding to the electron-gas like pair probability. According to the ELF results in Fig. S2, we can see that the ELF between B and B atoms in 2-D MnB is close to 1.0, indicating a strong covalent bonding character.

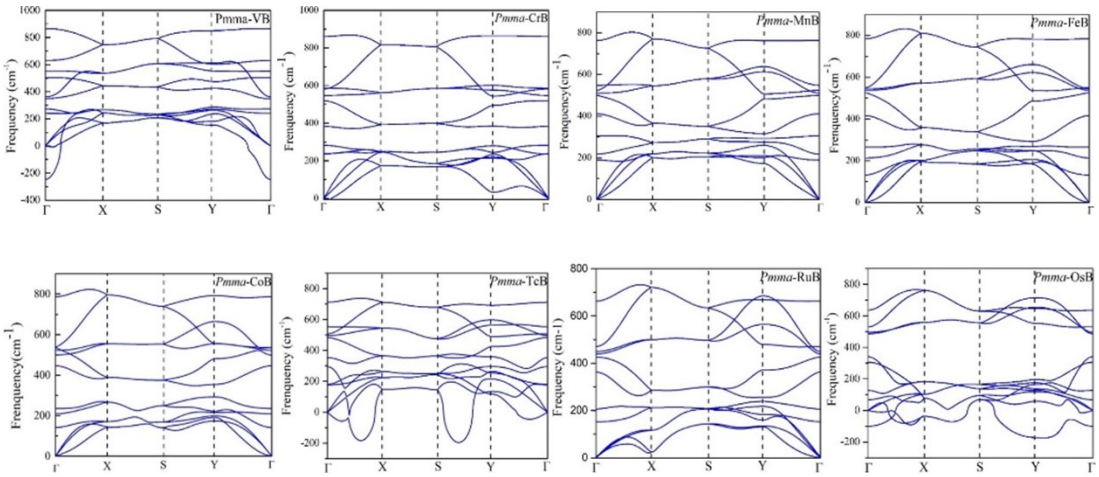


Fig. S3 Calculated phonon spectra of 2-D monolayer MBs using GGA-PBE.

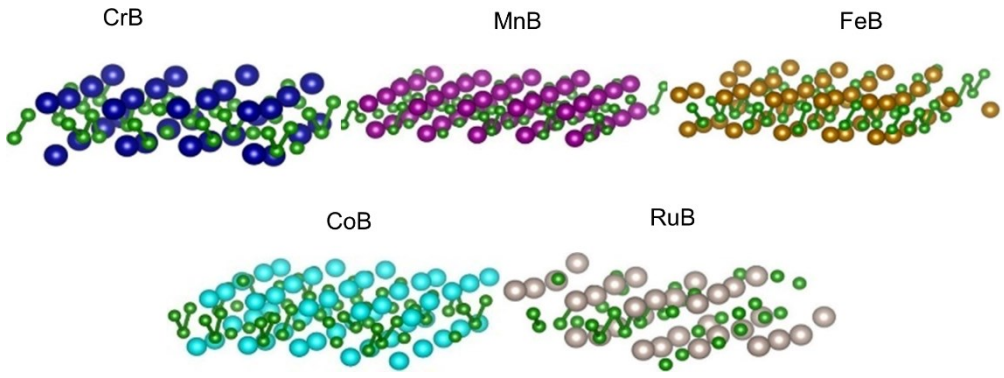


Fig. S4 Snapshots of 2-D monolayer MBs after 5 ps AIMD simulations at 600 K.

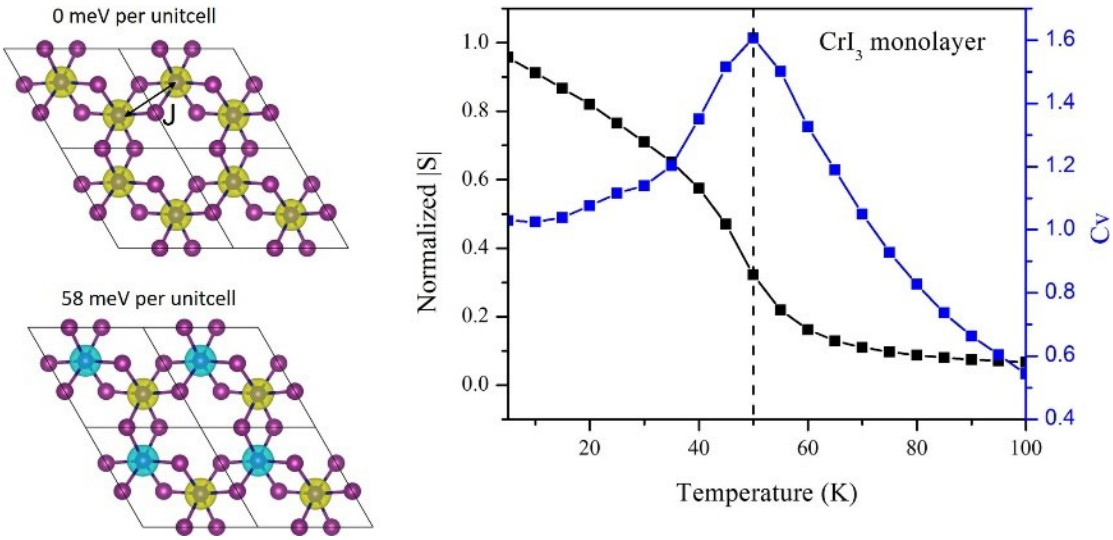


Fig. S5 Simulated normalized |S| (black data) and specific heat C_V (blue data) as a function of temperature for monolayer CrI_3.

For monolayer CrI_3, the energy difference between FM and AFM state per unit-cell is 58.0 meV. The J is obtained by $(E_{AFM}-E_{FM})/6S^2$, where **S** is the spin vector of each Cr atom. Using the normalized $|\mathbf{S}|=1$, J is 9.6 meV, which agrees with the value of 9.1 meV in same approach[S2]. The Curie temperature is about 50 K in Fig. S5.

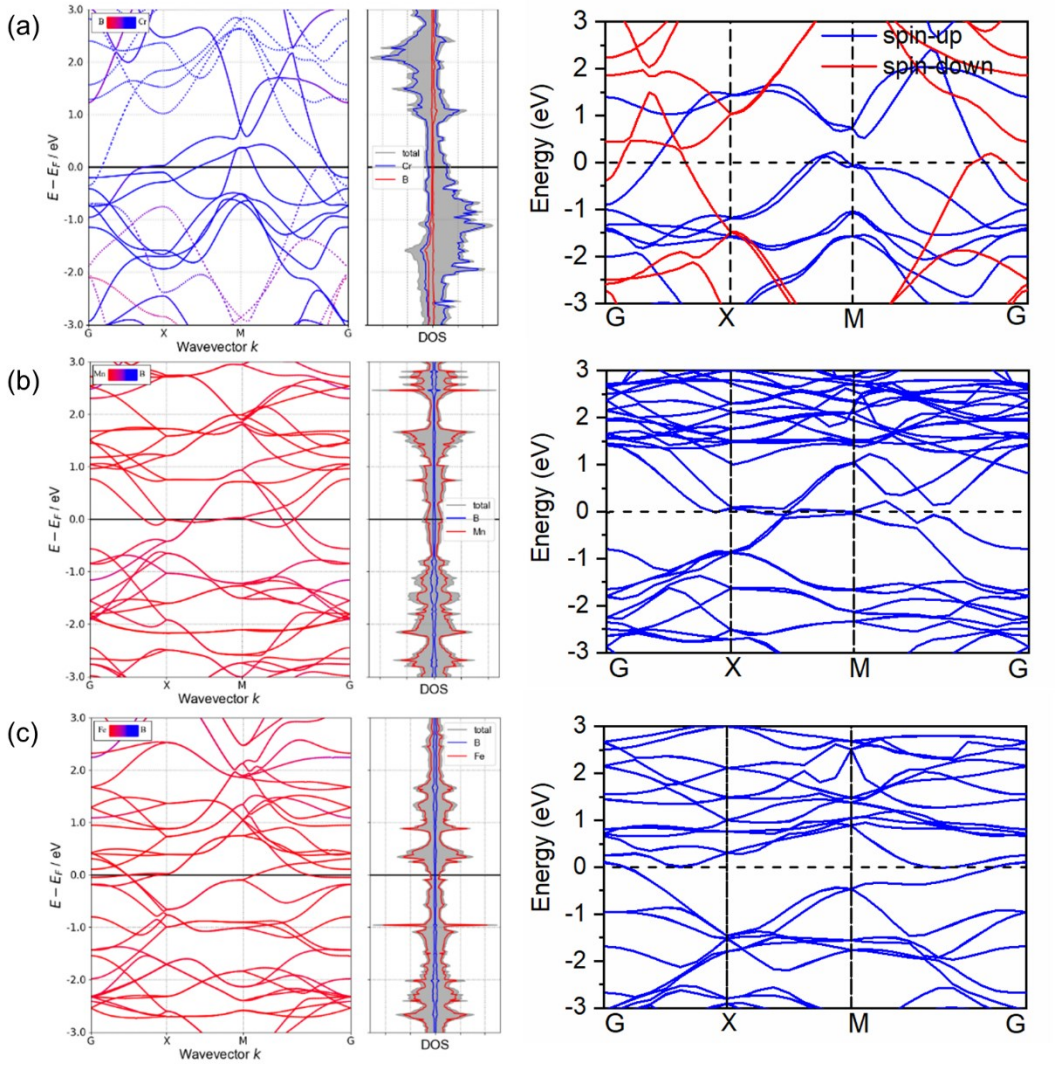


Fig. S6 Calculated band structure of 2-D (a) CrB, (b) MnB, and (c) FeB in their magnetic ground state by employing GGA+U (U_{eff} = 2.0 eV). The solid and dash lines respectively mean spin-up and spin-down channel. The contribution of DOS for each 2-D MB around the Fermi level are from transition-metal M atoms. Calculated band structure of 2-D (d) CrB, (e) MnB, and (f) FeB in their magnetic ground state by employing hybrid HSE06. The Fermi levels are set to zero. For the band structures of 2-D MnB and FeB, only the spin-up state is shown here. The figures (a), (b), and (c) are plotted by pymatgen.[S3]

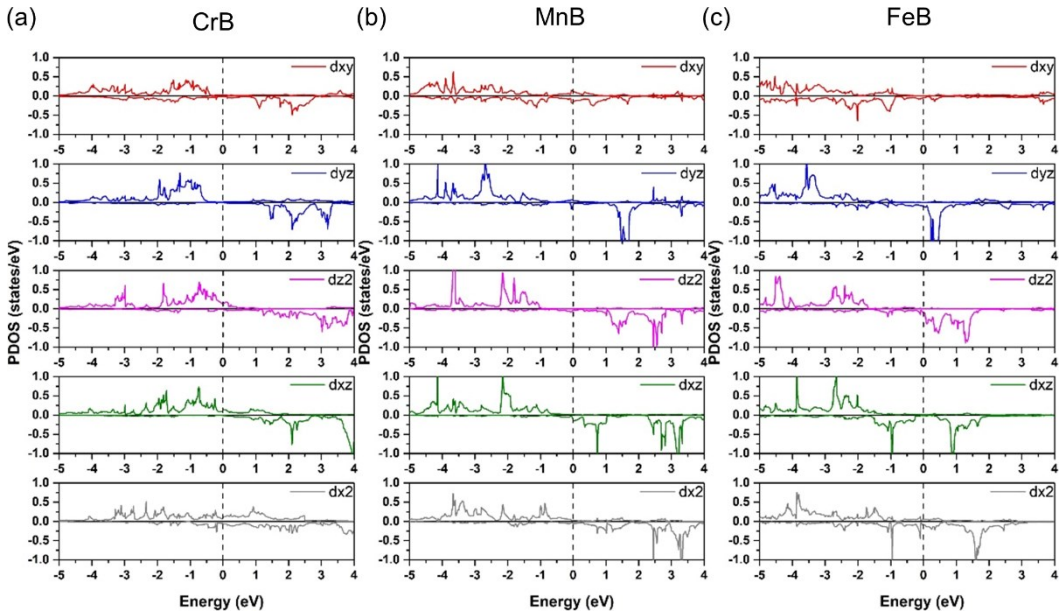


Fig. S7 Projected density of state (PDOS) of d_{xy}, d_{yz}, d_{z^2}, d_{xz}, and $d_{x^2-y^2}$ of 2-D (a) CrB, (b) MnB, (c) FeB using GGA+U. (U_{eff} =2.0 eV). The Fermi levels are set to zero.

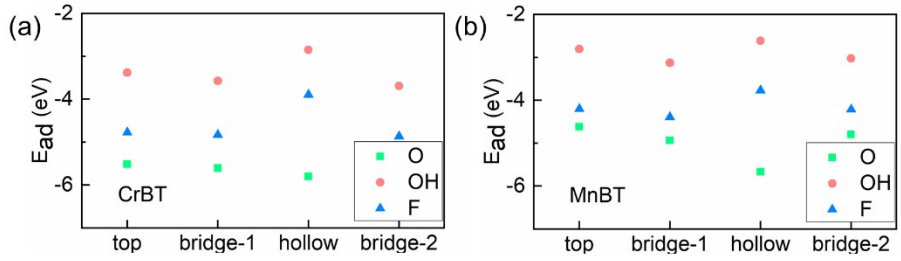


Fig. S8 Adsorption energies of different configurations of 2-D (a) CrBT and (b) MnBT. T is O, OH, and F respectively.

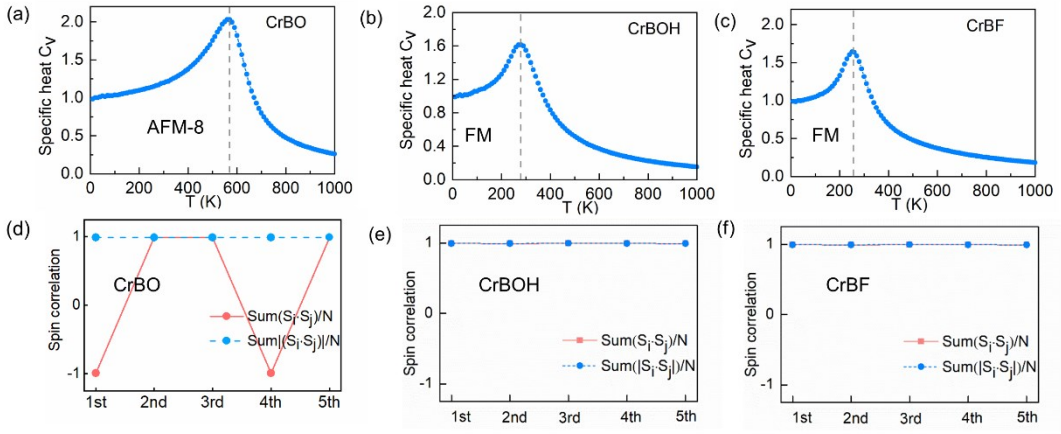


Fig. S9 Calculated specific heat C_V as functions of temperature T for 2-D (a) CrBO, (b)

CrBOH, and (c) CrBF. Calculated spin-spin correlations of 1st, 2nd, 3rd, 4th, and 5th neighboring magnetic atoms by Monte Carlo simulation at T=10 K for 2-D (d) CrBO, (e) CrBOH, and (f) CrBF.

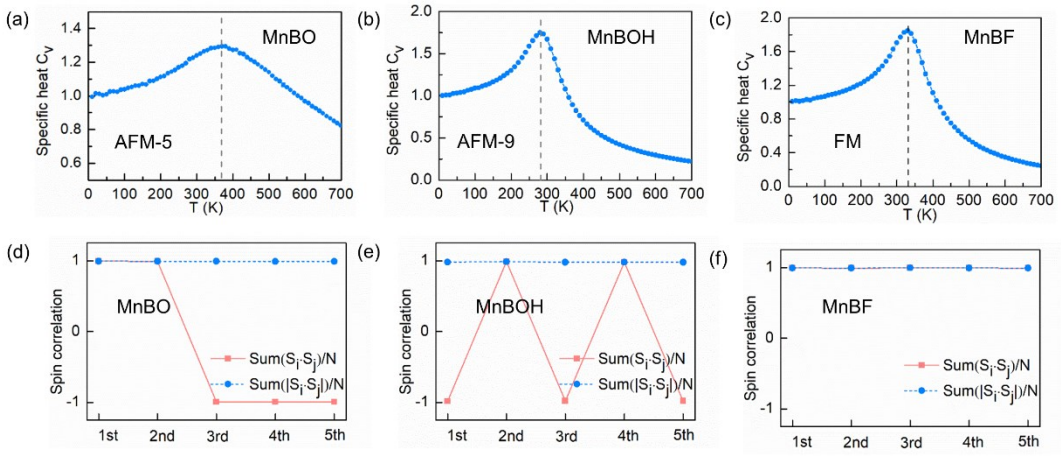


Fig. S10 Calculated specific heat C_V as functions of temperature T for 2-D (a) MnBO, (b) MnBOH, and (c) MnBF. Calculated spin-spin correlations of 1st, 2nd, 3rd, 4th, and 5th neighboring magnetic atoms by Monte Carlo simulation at T=10 K for 2-D (d) MnBO, (e) MnBOH, and (f) MnBF.

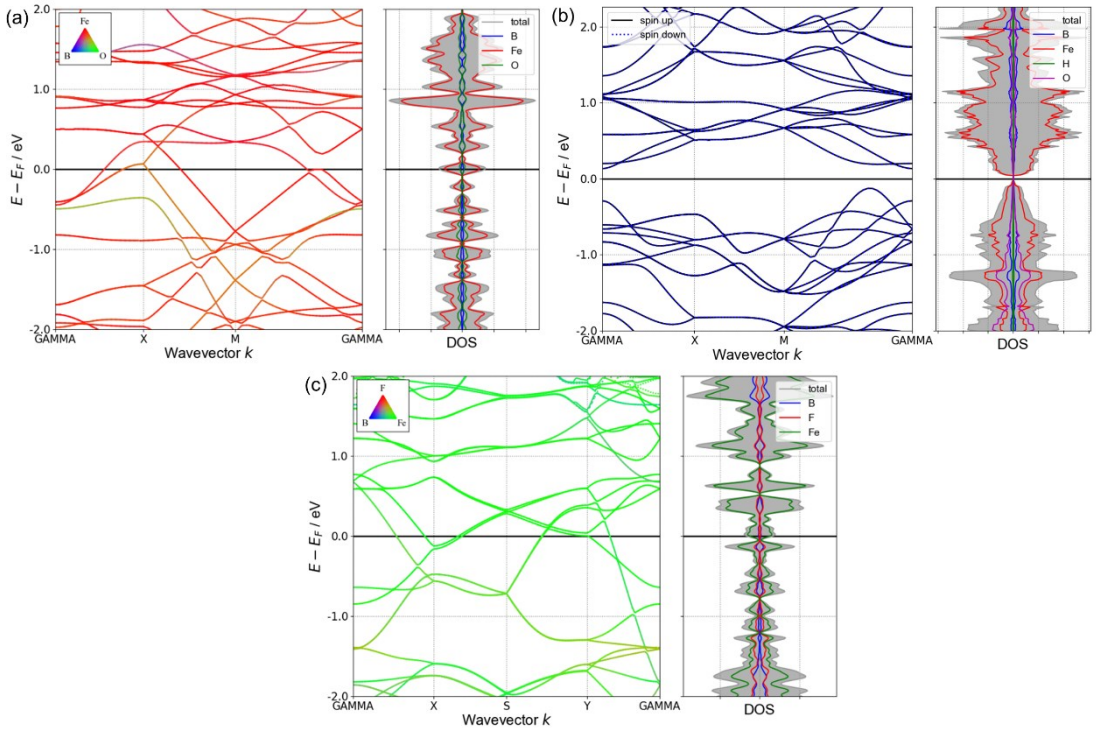


Fig. S11 Band structures and density of states (DOS) projected on each element for 2-D (a) FeBO, (b) FeBOH, and (c) FeBF, respectively both in most stable adsorption configuration and in magnetic ground state using GGA+U. The solid and dash line are respectively spin-up and spin-down state (U_{eff} = 2.0 eV). These figures are plotted by pymatgen.[S3]

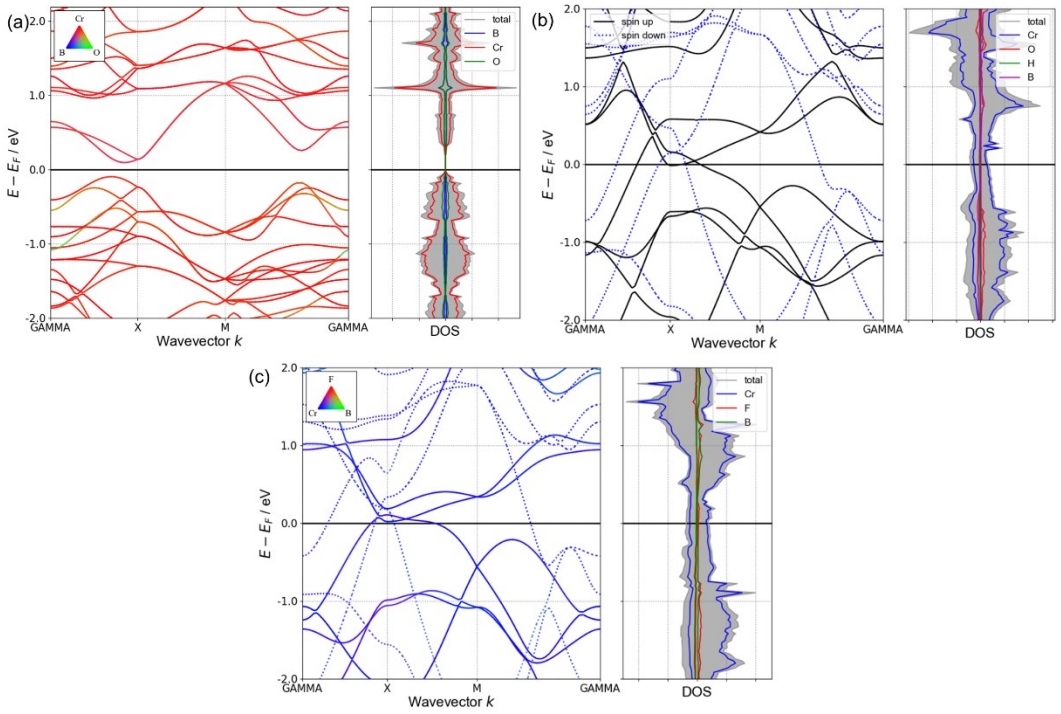


Fig. S12 Band structures and density of states (DOS) projected on each element for 2-D (a) CrBO, (b) CrBOH, and (c) CrBF, respectively both in most stable adsorption configuration and in magnetic ground state using GGA+U. The solid and dash line are respectively spin-up and spin-down state (U_{eff} = 2.0 eV). These figures are plotted by pymatgen.[S3]

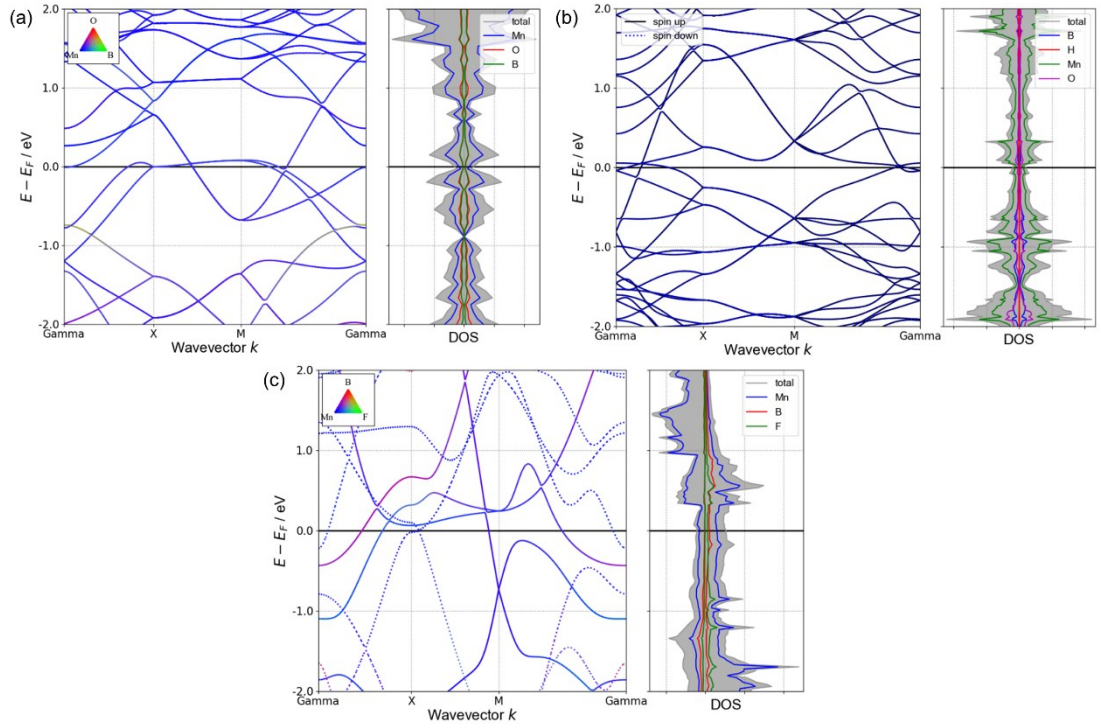


Fig. S13 Band structures and density of states (DOS) projected on each element for 2-D (a) MnBO, (b) MnBOH, and (c) MnBF, respectively both in most stable adsorption configuration and in magnetic ground state using GGA+U. The solid and dash line are respectively spin-up and spin-down state (U_{eff} = 2.0 eV). These figures are plotted by pymatgen.[S3]

From Fig. S11, S12, and S13, it is found that most of functionalized 2-D MBT (M = Fe, Mn, Cr; T = O, OH, F) are metallic with the Fermi energy falling into a continuum of energy states. However, for FeBOH and CrBO, the functionalized MBT are semiconductors with a small band gap of 0.26 or 0.19 eV, respectively.

Table S1. a and b (in Å) are lattice constant. l_1 and l_2 (in Å) are bond length between M and B atom. h (in Å) is layer height. M (in μB/f.u.) is the total magnetic moment per formula unit by using HSE06.

2-D *Pmma*	a	b	l_1	l_2	h	M
ScB	3.342	3.108	2.421	2.478	2.720	0.16
TiB	3.178	2.965	2.284	2.300	2.396	0.52
VB	3.264	2.901	2.206	2.223	1.906	1.94
CrB	2.948	2.879	2.211	2.157	2.290	3.20
MnB	2.928	2.881	2.172	2.116	2.118	3.50
FeB	2.803	2.832	2.147	2.052	2.119	2.75
CoB	2.644	2.911	2.102	2.034	2.156	1.59
NiB	2.584	2.917	2.170	2.053	2.393	0
YB	3.548	3.206	2.596	2.686	3.120	0.25
ZrB	3.291	3.089	2.434	2.481	2.825	0.12
NbB	3.208	3.001	2.351	2.356	2.573	0
MoB	3.052	3.045	2.274	2.252	2.338	0.68
TcB	3.019	3.015	2.295	2.196	2.250	1.29
RuB	2.911	2.971	2.298	2.177	2.425	1.05
RhB	2.761	2.976	2.345	2.192	2.724	0
PdB	2.919	2.996	2.362	2.246	2.678	0
HfB	3.242	3.068	2.404	2.441	2.765	0
TaB	3.183	2.969	2.353	2.339	2.593	0
WB	3.040	3.042	2.298	2.244	2.367	0.66
ReB	2.999	2.881	3.153	2.137	2.280	0
OsB	2.958	2.920	2.399	2.158	2.473	1
IrB	2.759	2.906	2.489	2.175	2.918	0
PtB	2.853	3.029	2.470	2.213	2.771	0

Table S2. Calculated elastic constants C (in GPa) of MBs, graphene, MoS_2 and Ti_2C monolayers. The data from other calculations[S4, S5, S6] are listed in parentheses for comparison. The cohesive energies E_{coh} (in eV) of 2-D MBs were obtained by using GGA.

2-D	C_{11}	C_{22}	C_{44}	C_{12}	E_{coh}
CrB	119.3	75.0	52.7	31.4	4.79
MnB	118.0	82.1	47.2	27.1	4.83
FeB	111.4	92.4	47.4	33.7	4.72
CoB	80.9	48.1	53.8	42.4	5.50
RuB	67.9	99.0	30.5	23.4	6.03
Graphene	351.6 (352.7)[4]	351.6 (352.7)[4]	145.4 (145.9)[4]	60.9 (60.9)[4]	/
MoS_2	131.1 (130)[5]	131.1 (130)[5]	49.3 (45)[5]	32.6 (40)[5]	/
Ti_2C	145.4 (137)[6]	145.4 (137)[6]	57.1 (53)[6]	31.2 (31.2)[6]	/

Table S3. E_{FM} and $E_{AFM\text{-}i}$ (in eV) are total energies of FM and AFM-i of 2-D MB (i=0, 1, 2, …,9) by using GGA+U (U_{eff} = 2.0 eV) and HSE06.

GGA+U	E_{FM}	$E_{AFM\text{-}0}$	$E_{AFM\text{-}1}$	$E_{AFM\text{-}2}$	$E_{AFM\text{-}3}$	$E_{AFM\text{-}4}$	$E_{AFM\text{-}5}$	$E_{AFM\text{-}6}$	$E_{AFM\text{-}7}$	$E_{AFM\text{-}8}$	$E_{AFM\text{-}9}$
FeB	-100.770	-101.330	-101.360	-101.420	-101.190	-101.399	**-101.820**	-101.460	-101.460	-101.380	-100.970
MnB	-108.634	-108.144	-108.667	-108.455	-108.370	-108.563	**-109.043**	-108.715	-108.571	-108.130	-107.795
CrB	**-109.780**	-109.400	-109.070	-108.730	-108.770	-109.141	-108.58	-108.500	-109.050	-109.190	-107.840
HSE06	E_{FM}	$E_{AFM\text{-}0}$	$E_{AFM\text{-}1}$	$E_{AFM\text{-}2}$	$E_{AFM\text{-}3}$	$E_{AFM\text{-}4}$	$E_{AFM\text{-}5}$	$E_{AFM\text{-}6}$	$E_{AFM\text{-}7}$	$E_{AFM\text{-}8}$	$E_{AFM\text{-}9}$
FeB	-147.220	-148.340	-148.500	-148.550	-148.480	-148.436	**-149.460**	-148.670	-148.540	-149.060	-148.510
MnB	-159.655	-158.300	-159.484	-159.031	-159.084	-158.839	**-160.174**	-159.588	-159.153	-159.133	-158.498
CrB	**-156.920**	-156.870	-156.100	-155.500	-155.600	-156.279	-155.160	-155.100	-156.460	-155.940	-154.050

Table S4. E_{FM} and E_{AFMi} (in eV) are total energies of FM and AFM-i by using different U_{eff} values for MnB, FeB, and CrB monolayers (i=0, 1, 2, …, 9).

FeB	E_{FM}	E_{AFM-0}	E_{AFM-1}	E_{AFM-2}	E_{AFM-3}	E_{AFM-4}	E_{AFM-5}	E_{AFM-6}	E_{AFM-7}	E_{AFM-8}	E_{AFM-9}
U_{eff}=1	-108.020	-108.230	-108.210	-108.240	-107.940	-108.192	**-108.670**	-108.190	-108.190	-107.830	-107.630
U_{eff}=2	-100.770	-101.330	-101.360	-101.420	-101.190	-101.399	**-101.820**	-101.460	-101.460	-101.380	-100.970
U_{eff}=3	-94.558	-95.201	-95.207	-95.082	-95.256	-95.2687	**-95.635**	-95.071	-95.363	-95.602	-95.238
U_{eff}=4	-88.749	-89.748	-89.711	-89.326	-89.645	-89.8401	-89.974	-89.606	-90.055	**-90.381**	-90.147
U_{eff}=5	-83.776	-84.887	-84.871	-84.554	-84.969	-85.0853	-84.888	-84.838	-84.876	**-85.634**	-85.546
MnB	E_{FM}	E_{AFM-0}	E_{AFM-1}	E_{AFM-2}	E_{AFM-3}	E_{AFM-4}	E_{AFM-5}	E_{AFM-6}	E_{AFM-7}	E_{AFM-8}	E_{AFM-9}
U_{eff}=1	**-114.960**	-114.636	-114.792	-114.778	-114.570	-114.945	-114.937	-114.750	-114.754	-114.147	-113.949
U_{eff}=2	-108.634	-108.144	-108.667	-108.455	-108.370	-108.563	**-109.043**	-108.715	-108.571	-108.130	-107.795
U_{eff}=3	-103.126	-102.382	-102.210	-102.835	-102.862	-102.828	**-103.740**	-103.294	-103.088	-102.827	-102.332
U_{eff}=4	-98.223	-97.226	-98.297	-97.804	-97.942	-97.709	**-98.940**	-98.386	-98.169	-98.090	-97.452
U_{eff}=5	-93.841	-92.634	-93.848	-93.268	-93.510	-93.155	**-94.583**	-93.935	-93.702	-93.823	-93.078
CrB	E_{FM}	E_{AFM-0}	E_{AFM-1}	E_{AFM-2}	E_{AFM-3}	E_{AFM-4}	E_{AFM-5}	E_{AFM-6}	E_{AFM-7}	E_{AFM-8}	E_{AFM-9}
U_{eff}=1	**-116.530**	-116.000	-115.730	-115.490	-115.690	-115.698	-115.460	-115.490	-115.620	-115.930	-115.150
U_{eff}=2	**-109.780**	-109.400	-109.070	-108.730	-108.770	-109.141	-108.580	-108.500	-109.050	-109.190	-107.840
U_{eff}=3	**-103.850**	-103.670	-103.200	-102.710	-102.740	-103.365	-102.380	-102.370	-103.470	-103.230	-101.320
U_{eff}=4	-98.518	**-98.590**	-97.953	-97.380	-97.492	-98.247	-96.921	-97.103	-98.455	-97.946	-95.600
U_{eff}=5	-93.628	**-94.028**	-93.234	-92.652	-92.800	-93.6865	-91.971	-92.455	-93.936	-93.212	-90.820

Table S5. Calculated magnetic couple constants of J_1, J_2, J_3, J_4, J_5 (in meV) and the critical temperature of T by using GGA+U.

2-D	Ground state	J_1	J_2	J_3	J_4	J_5	T_c
FeB	AFM-5	8.7	-10.0	-14.3	-21.9	-3.7	320
MnB	AFM-5	53.0	-2.6	-16.5	-12.4	5.7	300
CrB	FM	42.5	-21.5	52.4	-2.7	14.6	440

To obtain the strength of magnetic coupling of monolayer MB based on 2-D Heisenberg model, the energy in FM and collinear AFM-i (i=0, 1, …, 9) states were used to compute J_1, J_2, J_3, J_4, and J_5 using least-squares method. The equation (2) can be further written as:

$$E_{FM} = E_0 - 8J_1|S|^2 - 8J_2|S|^2 - 8J_3|S|^2 - 16J_4|S|^2 - 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-0} = E_0 + 0J_1|S|^2 + 8J_2|S|^2 - 8J_3|S|^2 + 0J_4|S|^2 + 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-1} = E_0 + 0J_1|S|^2 + 0J_2|S|^2 + 0J_3|S|^2 + 8J_4|S|^2 + 0J_5|S|^2 - A|S|^2$$

$$E_{AFM-2} = E_0 + 0J_1|S|^2 + 0J_2|S|^2 + 0J_3|S|^2 + 0J_4|S|^2 + 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-3} = E_0 + 4J_1|S|^2 + 0J_2|S|^2 + 0J_3|S|^2 + 0J_4|S|^2 + 0J_5|S|^2 - A|S|^2$$

$$E_{AFM-4} = E_0 + 0J_1|S|^2 + 8J_2|S|^2 + 0J_3|S|^2 + 0J_4|S|^2 + 0J_5|S|^2 - A|S|^2$$

$$E_{AFM-5} = E_0 - 8J_1|S|^2 - 8J_2|S|^2 + 8J_3|S|^2 + 16J_4|S|^2 + 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-6} = E_0 + 0J_1|S|^2 + 0J_2|S|^2 + 8J_3|S|^2 + 0J_4|S|^2 + 0J_5|S|^2 - A|S|^2$$

$$E_{AFM-7} = E_0 + 0J_1|S|^2 + 8J_2|S|^2 + 8J_3|S|^2 + 0J_4|S|^2 - 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-8} = E_0 + 8J_1|S|^2 - 8J_2|S|^2 - 8J_3|S|^2 + 16J_4|S|^2 - 16J_5|S|^2 - A|S|^2$$

$$E_{AFM-9} = E_0 + 8J_1|S|^2 - 8J_2|S|^2 + 8J_3|S|^2 - 16J_4|S|^2 + 16J_5|S|^2 - A|S|^2$$

where E_0 is the energy of the nonmagnetic state, J_1, J_2, J_3, J_4, and J_5 are the 1st, 2nd, 3rd, 4th, and 5th neighbor exchange coupling parameters, respectively. A is anisotropy energy parameter, which is obtained by using the magnetic anisotropy energy as:

$$A = \frac{E_{hard}(axis) - E_{easy}(axis)}{|S|^2}$$

Table S6. Magnetic anisotropy energy (MAE) is defined as the energy difference between the system with spin direction along the magnetic hard axis and the system

with spin parallel to the magnetic easy axis. K_1 and K_2 are anisotropy constants.

2-D	MAE	$K_{1(a-c)}$	$K_{2(a-c)}$	$K_{1(b-c)}$	$K_{2(b-c)}$	Easy axis
FeB	482.2	482.2	3.3	230.1	-0.1	c
MnB	222.7	222.7	-0.1	187.9	-0.3	c
CrB	23.6	20.2	-2.9	-6.5	0.04	b

Table S7. E_{FM} and E_{AFMi} (in eV) are total energies of FM and AFM-i of 2-D MBT (M= Fe, Mn, Cr; T= O, OH, F; i= 0, 1, 2, …,9) by using the GGA+U (U_{eff} = 2.0 eV). The slash means that the AFM configuration could not be retained and turns out to be nonmagnetic configuration after DFT calculations.

MBT	E_{FM}	E_{AFM-0}	E_{AFM-1}	E_{AFM-2}	E_{AFM-3}	E_{AFM-4}	E_{AFM-5}	E_{AFM-6}	E_{AFM-7}	E_{AFM-8}	E_{AFM-9}
FeBO	-160.997	-158.882	-159.697	/	-158.858	-159.498	**-161.605**	-159.860	-159.615	-157.854	-158.296
FeBOH	-186.145	-184.189	/	/	-185.729	/	-186.020	-185.917	-185.424	-185.782	**-187.076**
FeBF	-138.292	-138.043	-138.368	-138.649	-138.333	-138.460	-139.036	-138.912	-138.722	-137.449	**-139.173**
MnBO	-173.38	-172.45	-172.35	-172.68	-172.12	-172.35	**-173.50**	-172.42	-171.96	-171.39	-172.37
MnBOH	-196.16	-195.56	-195.71	-195.92	-195.84	-195.41	-196.16	-195.52	-195.15	-196.09	**-196.32**
MnBF	**-150.59**	-149.94	-149.94	-150.17	-150.06	-149.76	-150.31	-149.68	-149.3	-150.23	-150.37
CrBO	-174.061	-173.987	-174.448	/	-174.194	-174.315	-173.822	-174.103	-174.942	**-175.056**	-172.775
CrBOH	**-199.573**	-199.182	-199.028	/	-198.876	-199.323	-198.552	-198.929	-199.128	-198.430	-197.985
CrBF	**-152.141**	-151.772	-151.515	/	-151.338	-151.954	-151.042	-151.459	-151.880	-150.849	-150.334

Table S8. Magnetic couple constants J_1, J_2, J_3, J_4, J_5 (in meV), magnetic anisotropy energy MAE (μeV/atom), magnetic easy axis, and critical temperature T_c (in K) of 2-D

MBT by employing GGA+U (U_{eff} = 2.0 eV).

MBT	J_1	J_2	J_3	J_4	J_5	MAE	Ground state	Magnetic easy axis	T_c
FeBO	199.9	21.6	-39.3	-3.6	3.3	80.6	AFM-5	c	910
FeBOH	-21.7	75.9	-40.6	22.2	2.4	568.4	AFM-9	c	930
FeBF	22.5	4.8	-59.1	15.0	-9.3	720.6	AFM-9	c	420
MnBO	96.6	25.3	-1.0	13.4	-16.1	128.3	AFM-5	b	370
MnBOH	-3.8	50.8	12.7	3.8	-8.9	184.4	AFM-9	a	280
MnBF	8.1	44.4	25.3	6.7	-9.5	285.5	FM	c	330
CrBO	1.3	-30.5	9.5	-32.0	34.6	214.6	AFM-8	a	560
CrBOH	51.7	-36.9	21.6	8.1	11.1	37.3	FM	a	280
CrBF	61.4	-49.2	19.5	8.6	14.7	67.2	FM	a	250

The code for calculating *J* by using least-square method is as follow. Here, we take 2-D MnBO as an example.

```
Y= [-173.3776239 -172.4498714 -172.3529803 -172.683568 -172.1228168 -172.3525338 -173.4971323 -172.4150622 -171.9597934 -171.3890329 -172.3670717]';
X= [1 -8 -8 -8 -16 -16;1 0 8 -8 0 16;1 0 0 0 8 0;1 0 0 0 0 16;1 4 0 0 0 0;1 0 8 0 0 0;1 -8 -8 8 16 16;1 0 0 8 0 0;1 0 8 8 0 -16; 1 8 -8 -8 16 -16;1 8 -8 8 -16 16];
B1_3 = pinv(X'*X)*X'*Y;
B2_3 = (X'*X)^-1*X'*Y;
B3_3 = [B1_3 B2_3]
Yp = X*B2_3;
err = [abs(Y-Yp)./Y]'
Ym = mean(Y);
SStot = sum((Y-Ym).^2);
SSreg = sum((Yp-Ym).^2);
SSres = sum((Yp-Y).^2);
R2 = 1-SSres/SStot
plot(Yp,Y,'o');
hold on
```

plot([min(Yp) max(Yp)],[min(Yp) max(Yp)])

hold off

The calculated results are as follow.

B3_3 = -172.4540 -172.4540

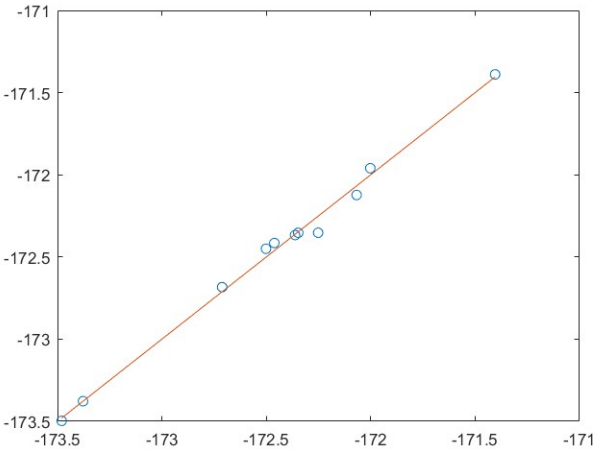
0.0966 0.0966

0.0253 0.0253

-0.0010 -0.0010

0.0134 0.0134

-0.0161 -0.0161



$R^2 = 0.994$

Therefore, the values of J_1, J_2, J_3, J_4, and J_5 of MnBO are respectively 96.6 meV, 25.3 meV, -1.0 meV, 13.4 meV, and -16.1 meV.

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