Exploring room-temperature ferromagnetism in WXBC (X=W, Mn, Fe) monolayers

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Linear response approach for Hubbard *U* parameter calculation:

We employed linear response approach proposed by Cococcioni *et al*. [1], as implemented in the Quantum Espresso package [2], to evaluate the U parameter for WXBC ($\mathrm{X = W, Mn, Fe}$) monolayers. As illustrated in Fig. S1, the non-interacting and interacting inverse matrix is the gradients of the bare and self-consistent regression response functions. The calculated U_{eff} values for WXBC monolayers are displayed in Fig. S1.

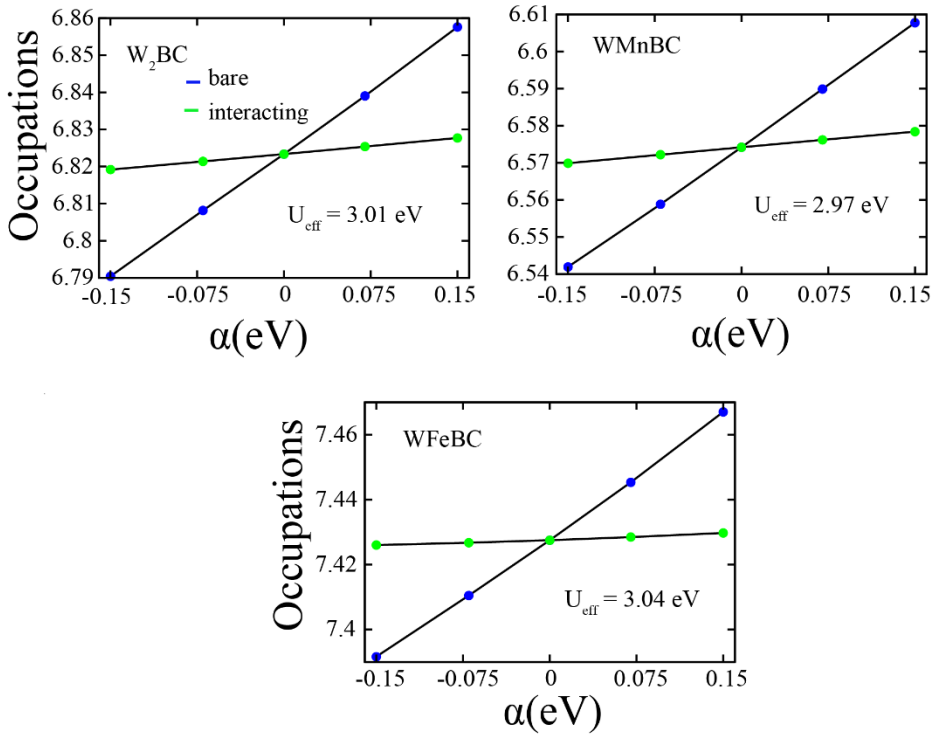

Figure S1: Linear response of d orbital occupations as a function of potential shift α. The curves depicted by the squares and circles lines are labelled bare and interacting. The inverse response

functions are deduced numerically by calculating the slope of the curves. $\varkappa_0$ follows from the slope of curve bare, whereas $\varkappa$ from the slope of curve interacting.

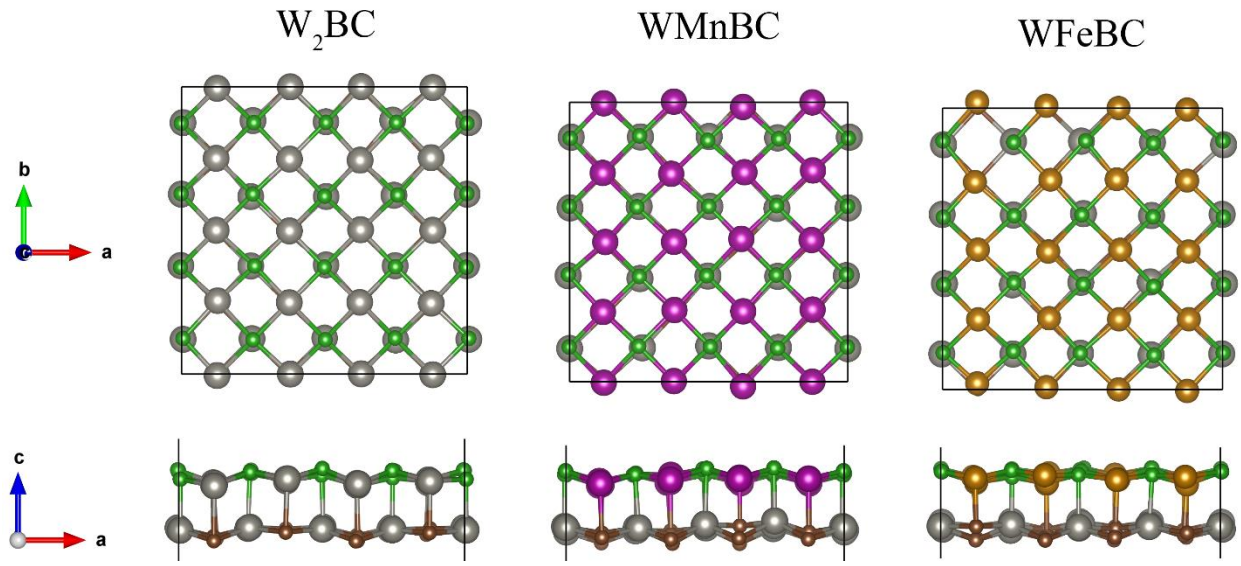

Figure S2: Top and side view 4× 4× 1 supercell of WXBC (X = W, Mn, Fe) monolayers under a Nose−Hoover thermostat at 300K with a time step of 3.0 fs.

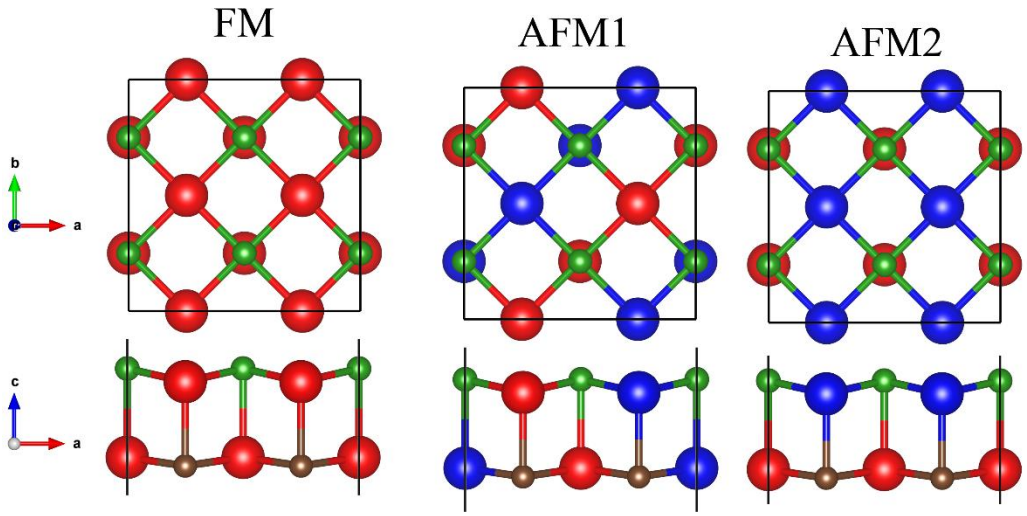

Figure S3. Top and side view views (a−c) of geometric structures of an (a) FM and two different (b) AFM1 (c) AFM2 states for WXBC (X = W, Mn, Fe) monolayers. Red and blue color denote the spin up and spin down respectively.

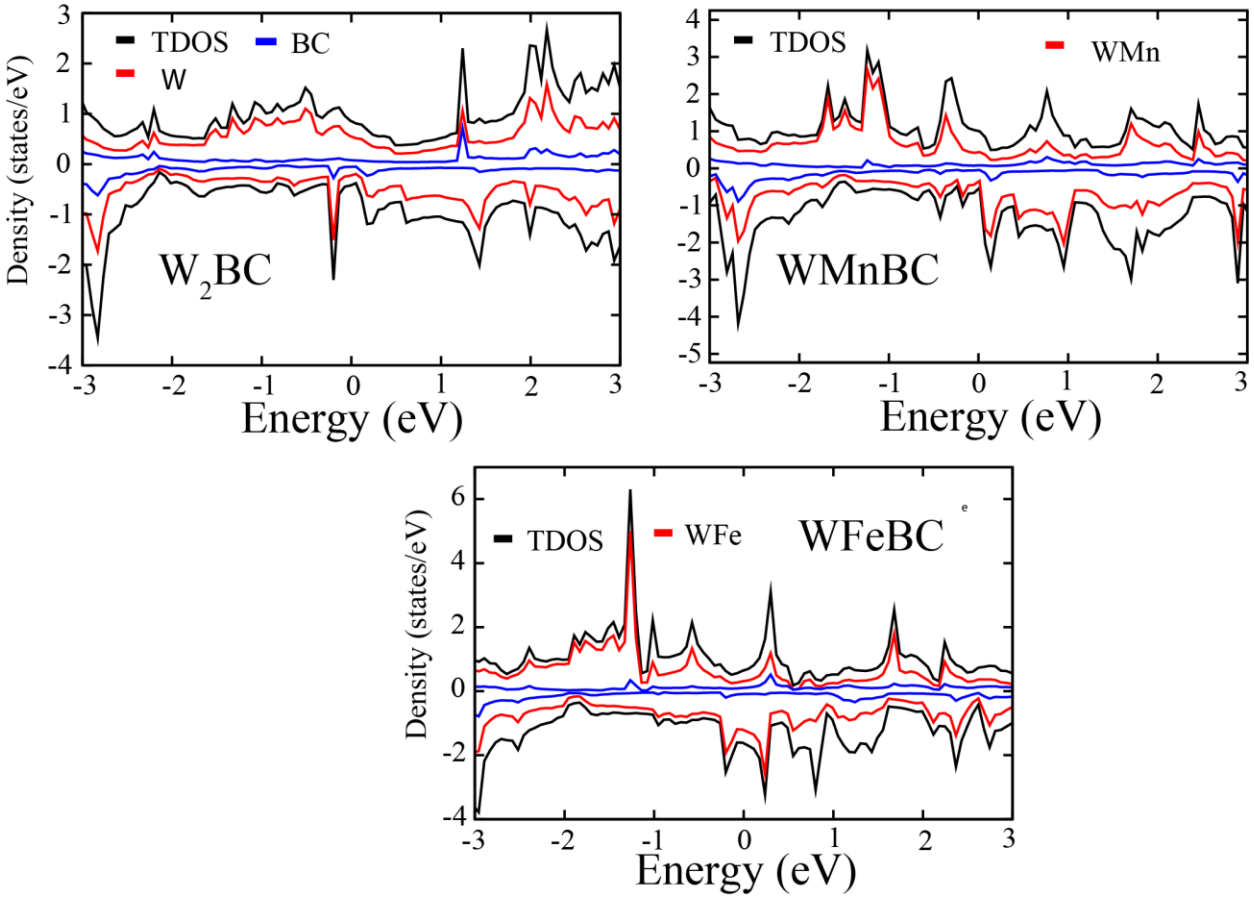

Figure S4. Total density of states (TDOS) for $WXBC$ $(X = W, Mn, Fe)$ monolayers.

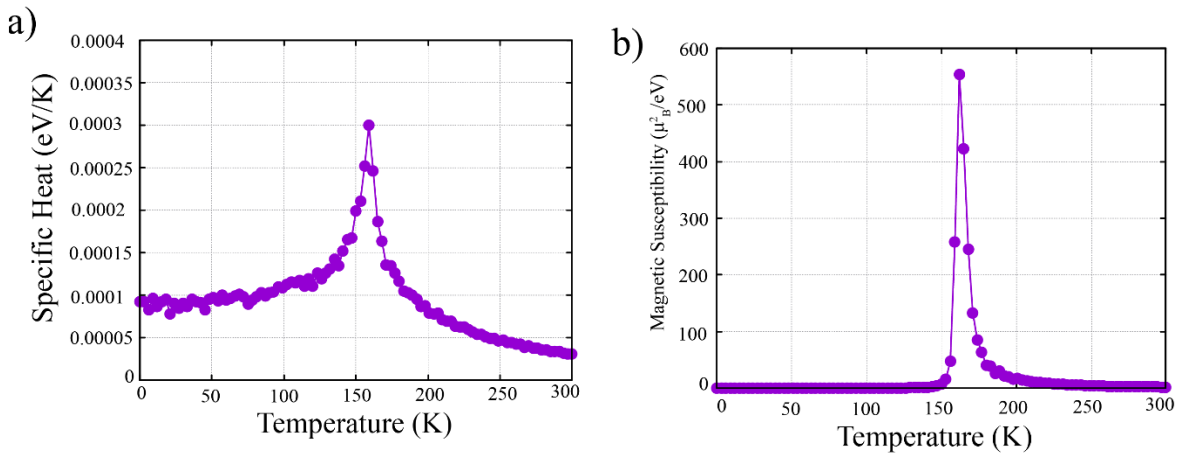

Figure S5. (a) Magnetic susceptibility and (b) Specific heat as a function of temperature for the W_2BC monolayer.

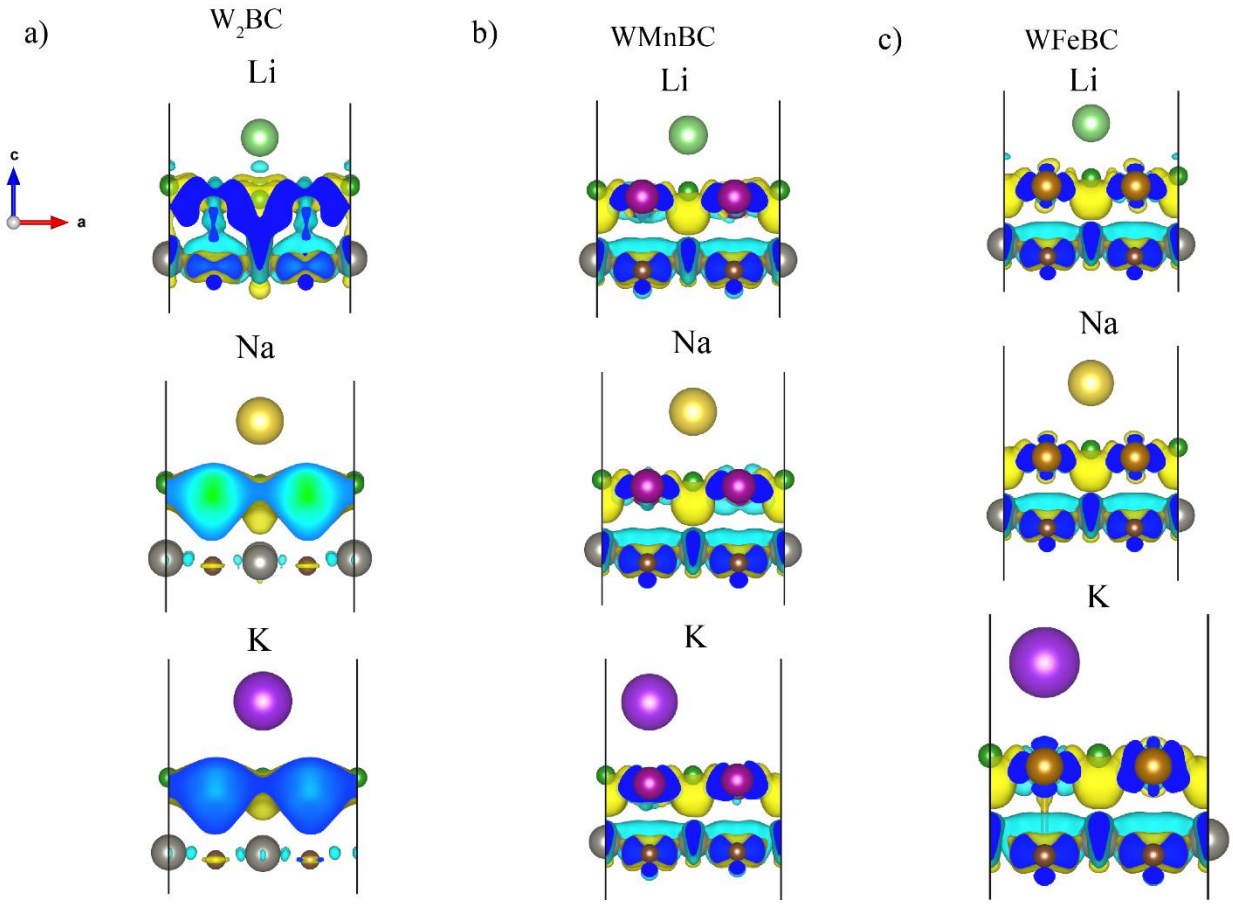

Figure S6. Charge density difference for atm@WXBC monolayers. Here, atm means adsorbed Li, Na and K atoms. The charge density difference maximum iso-surface values are approximately 0.036/0.130/0.130 e Å^{-3} for W2BC with adsorbed Li/Na/Ka systems, while those of WMnBC and WFeBC with adsorbed Li/Na/K cases are 0.037/0.041/0.037 e Å^{-3} and 0.047/0.044/0.050 e Å^{-3}, respectively.

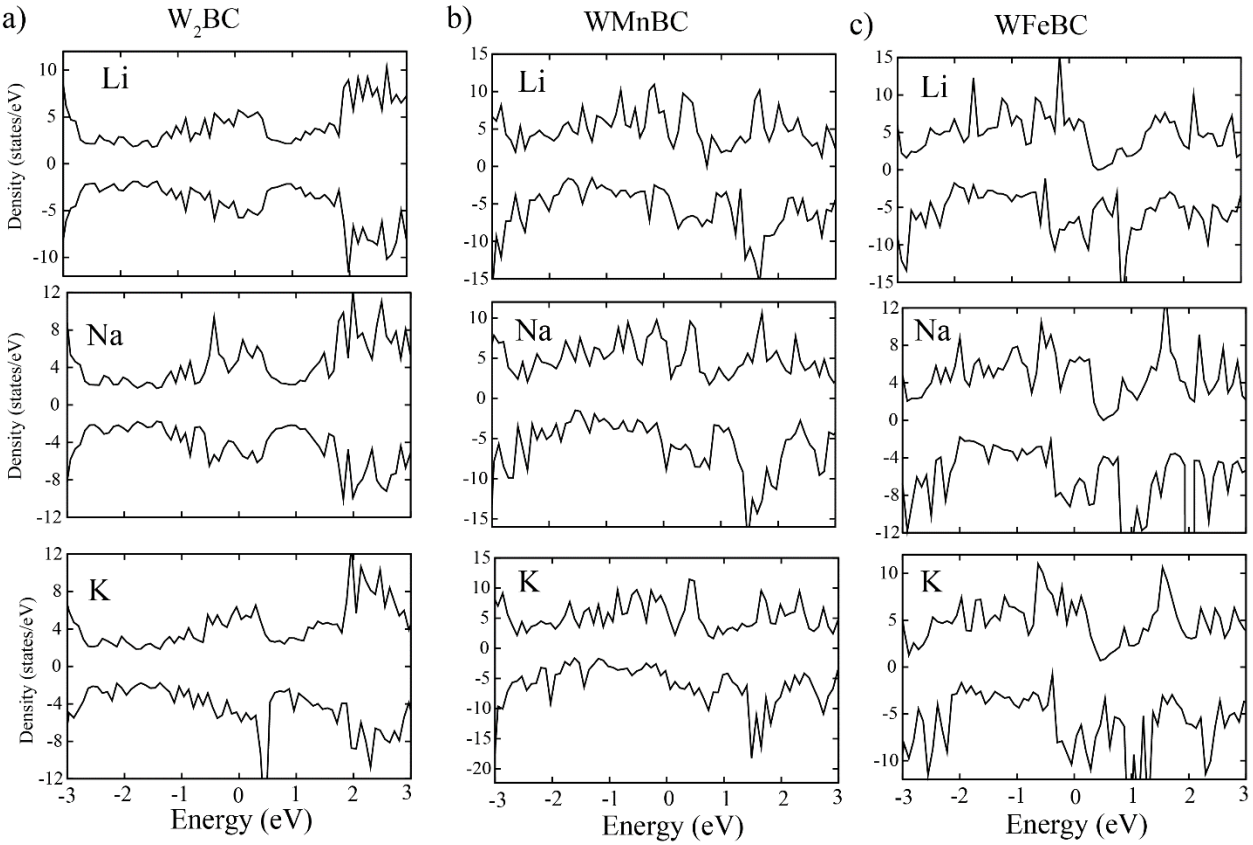

Figure S7. TDOS for atm@WXBC ($\mathrm{X} = \mathrm{W}, \mathrm{Mn}, \mathrm{Fe}$) structures. Here, atm means adsorbed Li, Na and K atoms.

Supporting Tables

Table S1. Cohesive energy, E_{coh}, formation energy, E_{FE} (in eV per atom), averaged bond lengths L_{xy}/L_z (Å) in the $x-y$ plane and z axis, in-plane stiffness Y (N/m), Poisson's ratio, ν, magnetic ordering, M and total magnetic moment, m_{T} (in μ_{B} per unit cell) for a series of WXBC ($\mathrm{X} = \mathrm{W}, \mathrm{Mn}, \mathrm{Fe}$) monolayers are listed. m is the magnetic moment of each magnetic ions in in μ_{B}.

System	W_2BC	WMnBC	WFeBC
E_{coh}	7.98	6.69	6.86
E_{FE}	-0.12	-0.03	0.03
$Y\ (a/b)$	210.63/210.63	153.56/153.70	208.93/216.09
$\nu\ (a/b)$	0.504/0.504	0.349/0.349	0.280/0.290
M	NM	FM	FM
m_{T} (PBE)	0	2.34	1.59
m_{T} (PBE+U)	1.15	2.28	1.72
m (PBE+U)	W(1.13, 0.33)	W(0.65), Mn(1.99)	W(0.50), Fe(1.51)

Table S2. Relative energies (eV) between FM and AFM for WXBC ($X = W, Mn, Fe$) monolayers.

System	FM	AFM1	AFM2
W_2BC	0	0.192	0.104
WMnBC	0	0.465	0.223
WFeBC	0	0.518	0.208

Table S3 (a): MAE Per unit cell in μeV for W_2BC monolayer. The easy axis (EA) is out of the plane [001] and FM as the ground state.

MAE	EA
$E(100) - E(001)$	9710
$E(010) - E(001)$	9710
$E(110) - E(001)$	8280
$E(111) - E(001)$	5410

Table S3 (b): MAE Per unit cell in μeV for WMnBC monolayer. The easy axis (EA) is within the basal plane [100] and FM as the ground state.

MAE	EA
$E(001) - E(100)$	1980
$E(010) - E(100)$	0
$E(110) - E(100)$	1260
$E(111) - E(100)$	1390

Table S3 (c): MAE Per unit cell in μeV for WFeBC monolayer. The easy axis (EA) is within the basal plane [100] and FM as the ground state.

MAE	EA
$E(001) - E(100)$	50
$\mathbf{E(010) - E(100)}$	**0**
$E(110) - E(100)$	160
$E(111) - E(100)$	150

Table S4 (a): MAE Per unit cell in μeV for W_2BC monolayer under electric field. The easy axis (EA) is out of the plane [001] and FM as the ground state.

Electric field (eV/Å)	$E(100) - E(001)$	$E(010) - E(001)$	$E(110) - E(001)$	$E(111) - E(001)$	EA
0	9710	9710	8280	5410	001
0.2	7070	7070	8940	5730	001
0.4	7090	7080	9100	6110	001
0.6	7010	7010	8520	5590	001
0.8	7390	7390	9050	6420	001
1.0	5330	5200	5090	4660	001

Table S4 (b): MAE Per unit cell in μeV for W_2BC monolayer under Biaxial Strain. The easy axis (EA) is out of the plane [001] and FM as the ground state.

Strain (%)	$E(100) - E(001)$	$E(010) - E(001)$	$E(110) - E(001)$	$E(111) - E(001)$	EA
-3	12500	12510	12510	8920	001
0	9710	9710	8280	5410	001
3	1050	1050	1570	1680	001
6	11760	11760	12110	7940	001

Table S5: Relative energies in eV between FM and AFM for WXBC ($X = W, Mn, Fe$) monolayers with adsorbed Li, Na and K atoms.

Sheet	Atoms	$E_{AFM} - E_{FM}$	Magnetic Ordering
W_2BC	Li	8.253	FM
	Na	8.348	FM
	K	8.203	FM
WMnBC	Li	6.083	FM
	Na	5.919	FM
	K	5.996	FM
	Li	5.927	FM

WFeBC	Na	5.977	FM
	K	6.099	FM

Table S6. Stable Ads. Site for Li, Na, K atoms. The adsorption energy (E_{ad}) and the adsorption height (h) i.e the distance between the W_2BC, $WMnBC$, and $WFeBC$ sheets and the adatoms (adsorbed Li, Na, K atoms). M_{cell} and EC denote the magnetic moment and electronic character of the $\mathrm{atm}-\mathrm{WX}BC$ $(X = W, Mn, Fe)$ systems with their corresponding magnetic ground state (GS_{M}). Charge transfer into the WXBC is denoted by Q. The electronic character (EC) of the $\mathrm{atm}-$ WXBC structures are all Metallic.

System	Adsorbate	Ads.	E_{ads} (eV)	h (Å)	Q (e-)	GS_{M}	M_{cell} (μ_{B})
W_2BC	Li	$\mathrm{T_B}$	8.64	2.03	0.84	FM	0.43
	Na	$\mathrm{T_B}$	8.73	2.40	0.73	FM	0.36
	K	$\mathrm{T_B}$	8.98	2.70	0.75	FM	0.71
$WMnBC$	Li	$\mathrm{T_H}$	6.71	2.29	0.86	FM	8.13
	Na	$\mathrm{T_H}$	6.60	2.65	0.76	FM	8.63
	K	$\mathrm{T_{Mn}}$	7.00	2.85	0.78	FM	8.00
$WFeBC$	Li	$\mathrm{T_H}$	6.82	2.31	0.86	FM	6.71
	Na	$\mathrm{T_H}$	6.76	2.63	0.77	FM	6.78
	K	$\mathrm{T_{Fe}}$	7.06	2.85	0.76	FM	7.22

References

[1] M. Cococcioni, S. De Gironcoli, Phys. Rev. B., 71 (2005) 035105.

[2] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G.L. Chiarotti, M. Cococcioni, I. Dabo, J. Phys. Condens. Matter., 21 (2009) 395502.