Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The intrinsic magnetism, quantum anomalous Hall effect and Curie temperature in 2D transition metal trihalides

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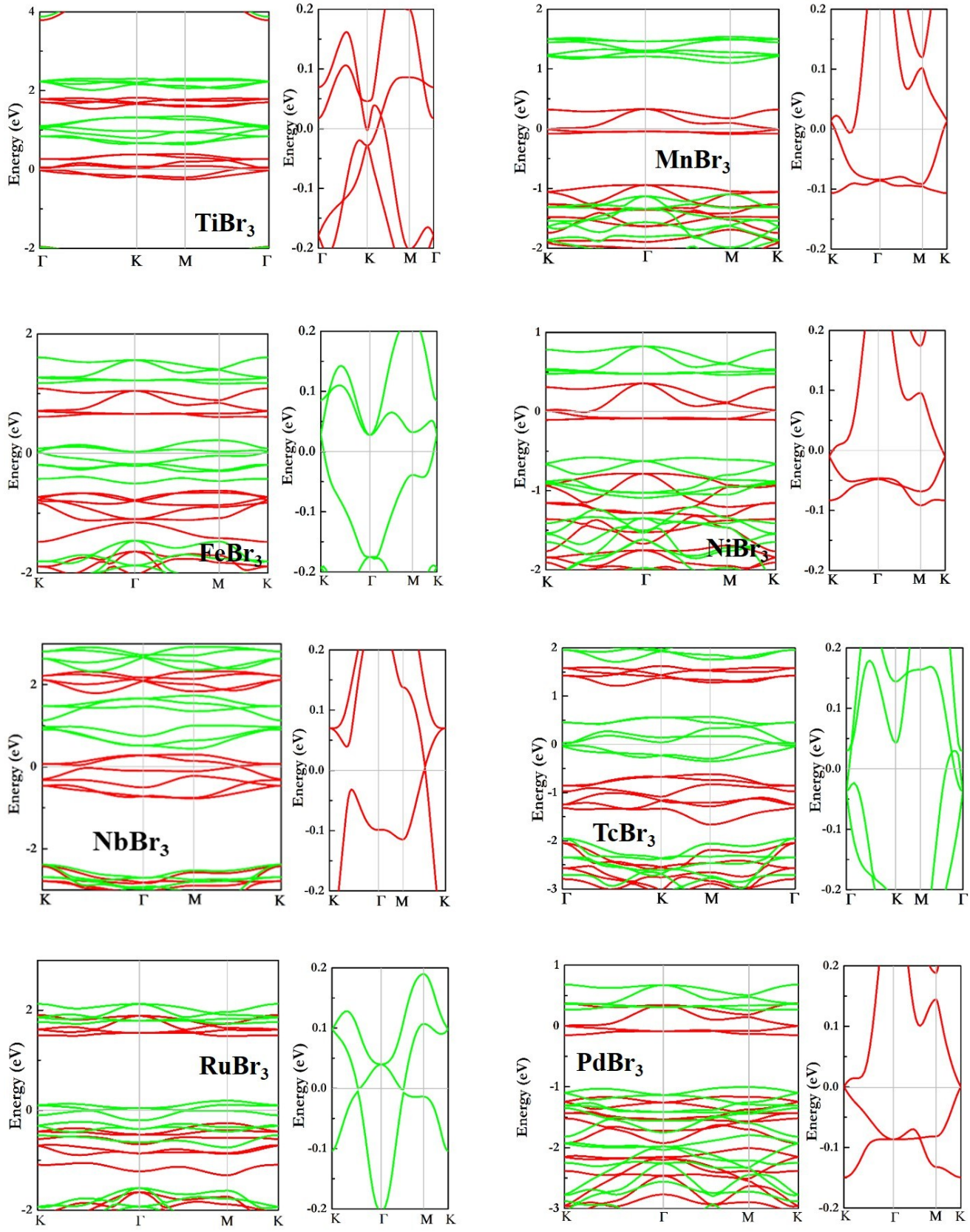

Figure S1. Spin-polarized band structure of transition metal tri-bromides obtained with the PBE functional. The spin-up bands and spin-down bands are shown in red and green, respectively.

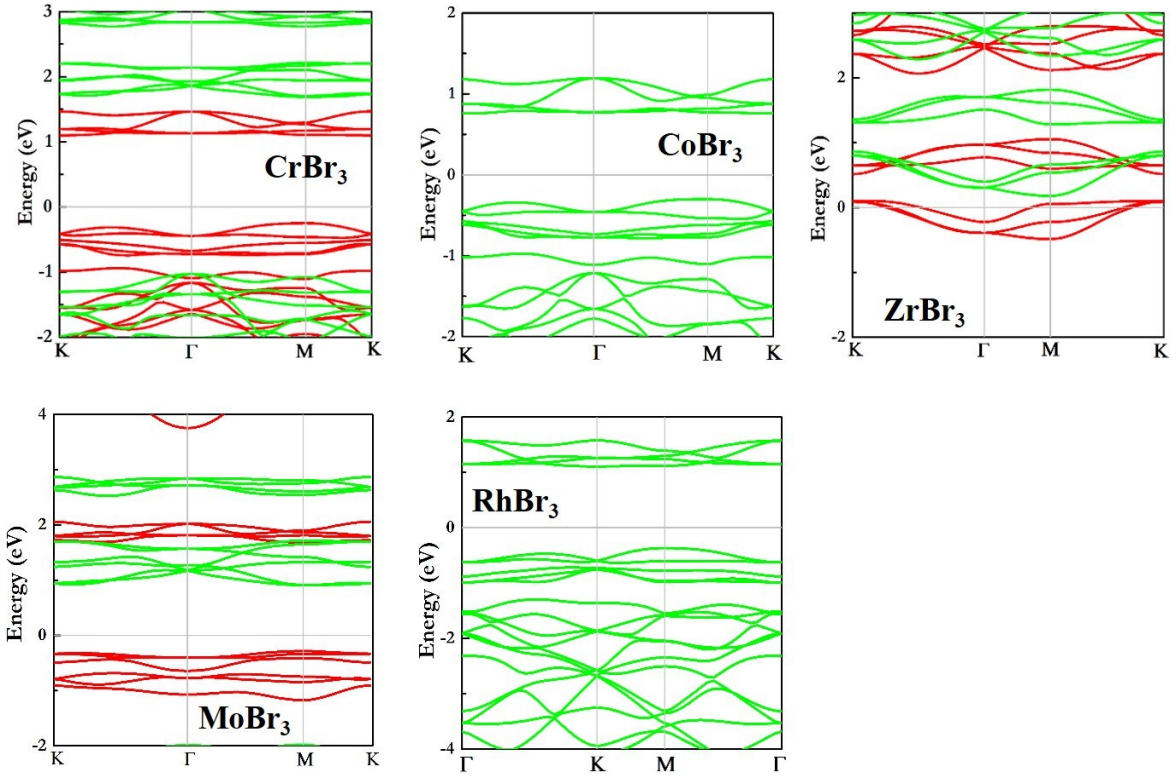

Figure S2. Spin-polarized band structure of transition metal tri-bromides obtained with the PBE functional. The spin-up bands and spin-down bands are shown in red and green, respectively. The $CoBr_3$ and $RhBr_3$ are nonmagnetic.

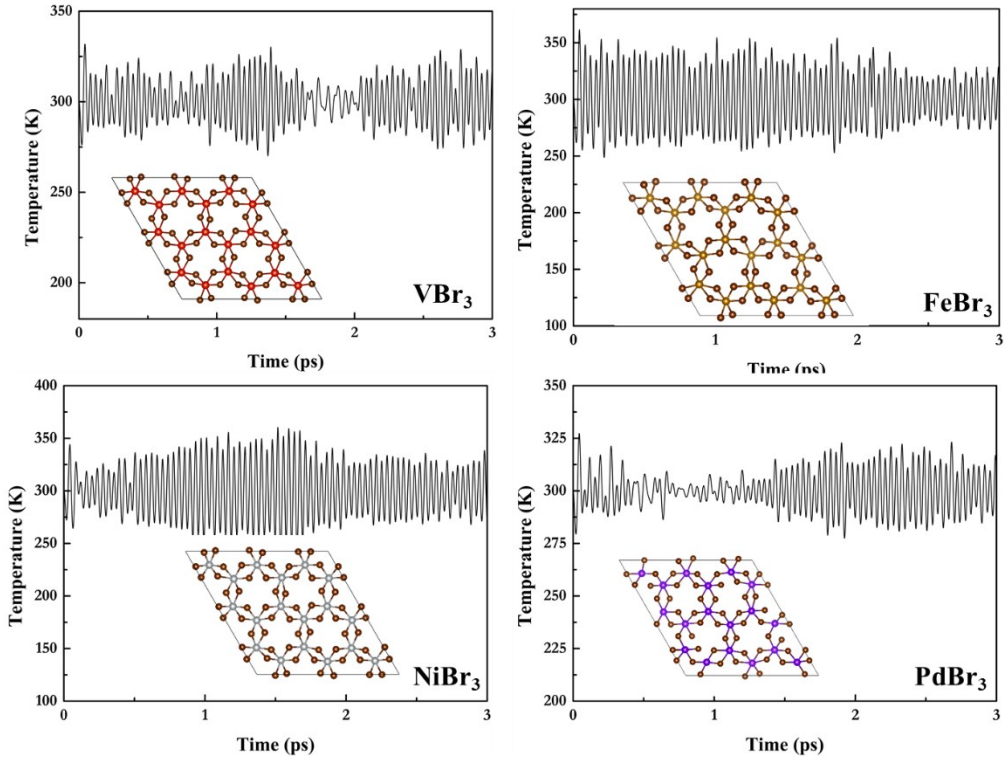

Figure S3. The fluctuation of potential energy (72 atoms/cell) as a function of AIMD simulation steps at 300 K calculated using PBE functional.

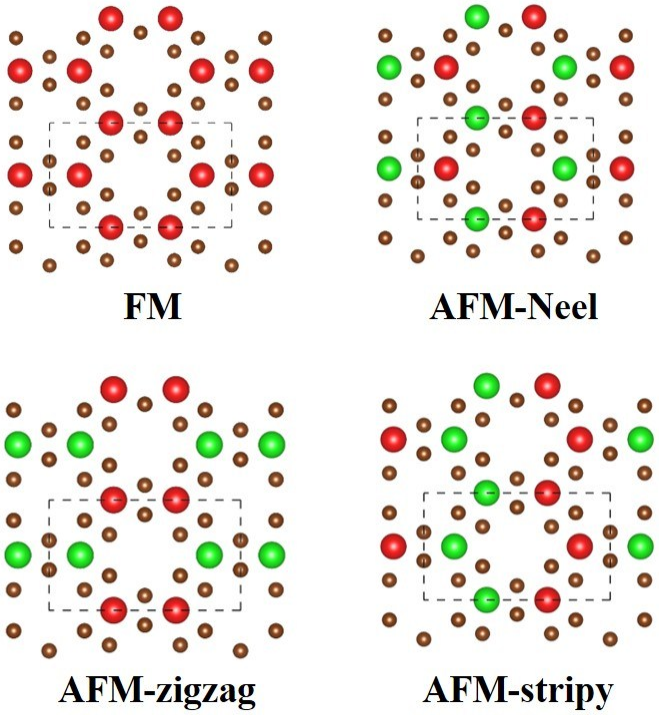

Figure S4. Possible configurations of V spins: (a) ferromagnet (FM), (b) Néel antiferromagnet (AFM- Néel), (c) stripy AFM, and (d) zigzag AFM.

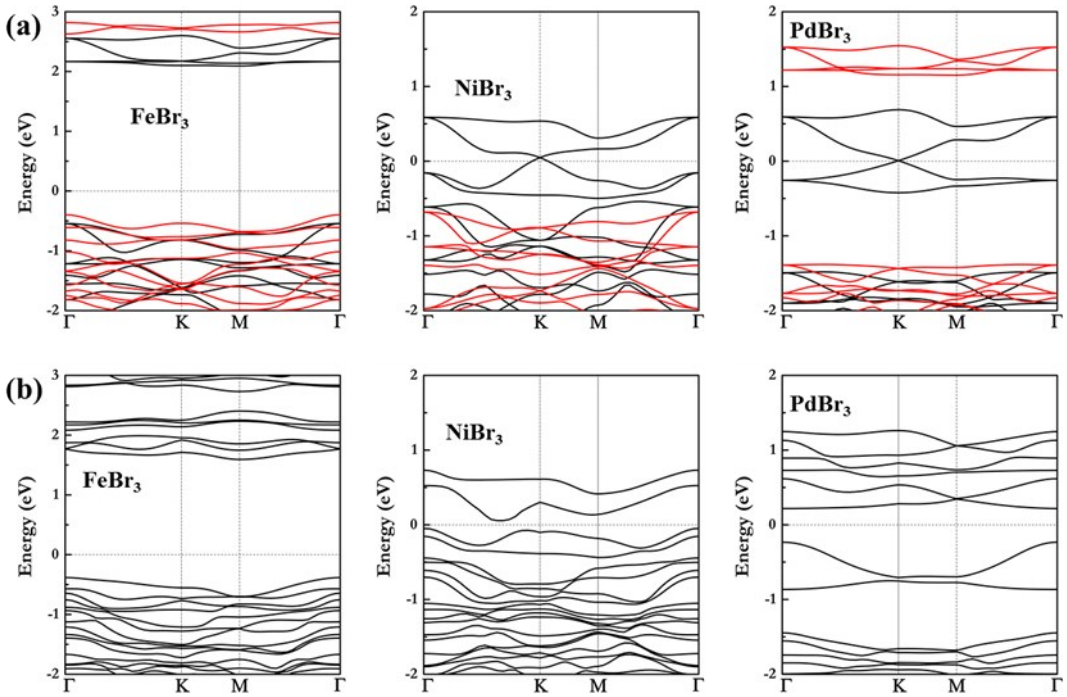

Figure S5. Spin-polarized band structures without (a) and with SOC (b) at HSE06 level. Inset: Dirac states near the Fermi level. The black and red lines represent the spin up and spin down channels, respectively.

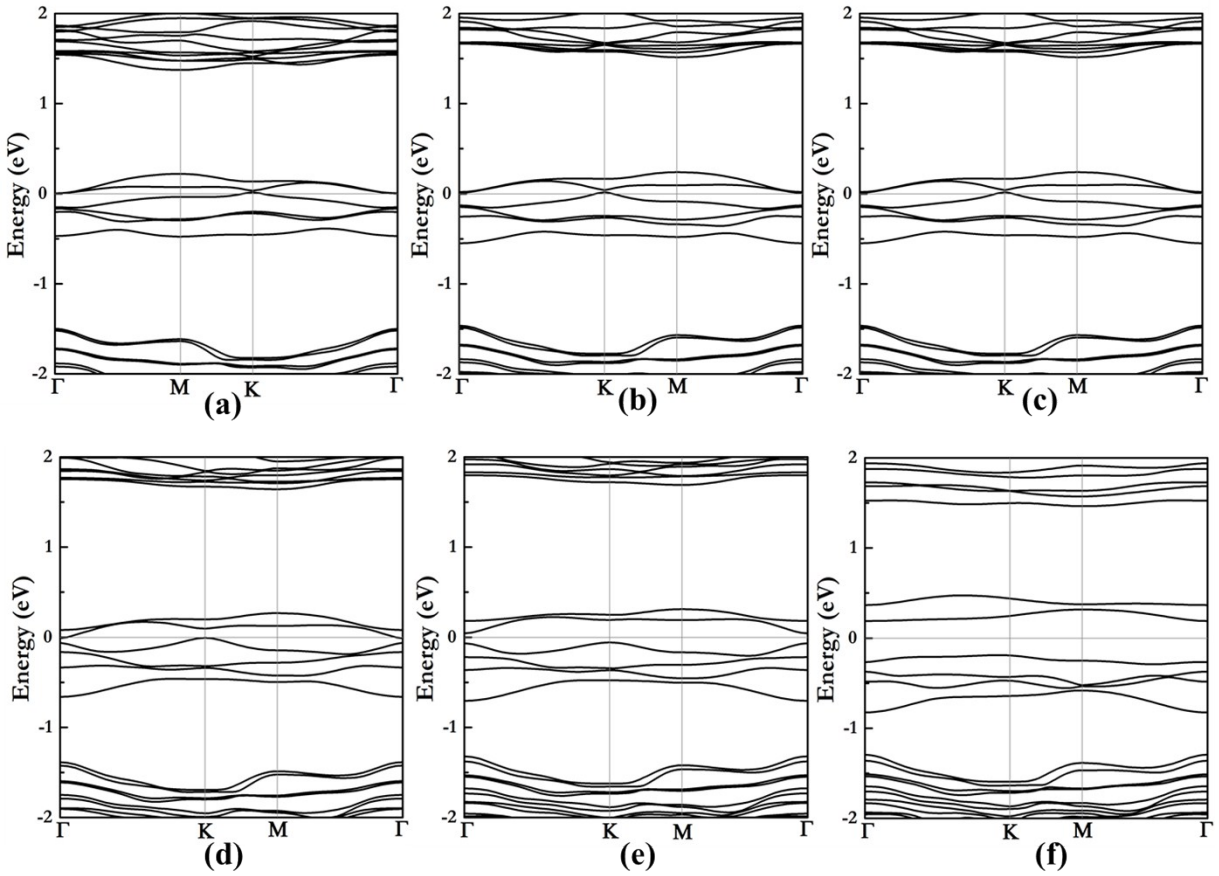

Figure S6. Band structures of VBr_3 calculated by GGA +U with SOC. (a) U=0.2 eV, (b) U=0.4 eV, (c) (d) U=0.6 eV, (e) U=0.8 eV, and (f) U=1.0 eV.

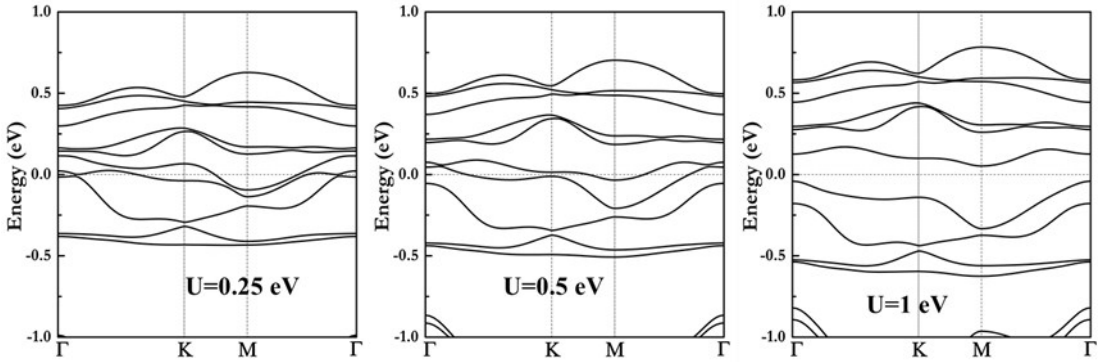

Figure S7. Band structures of $FeBr_3$ calculated by GGA +U with SOC.

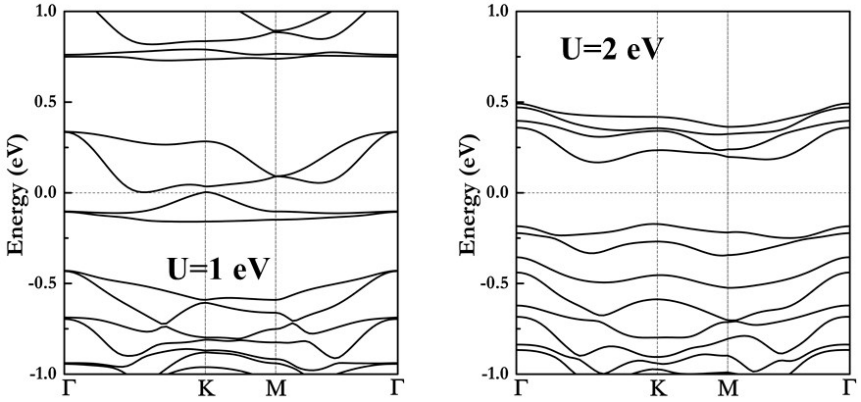

Figure S8. Band structures of $NiBr_3$ calculated by GGA +U with SOC.

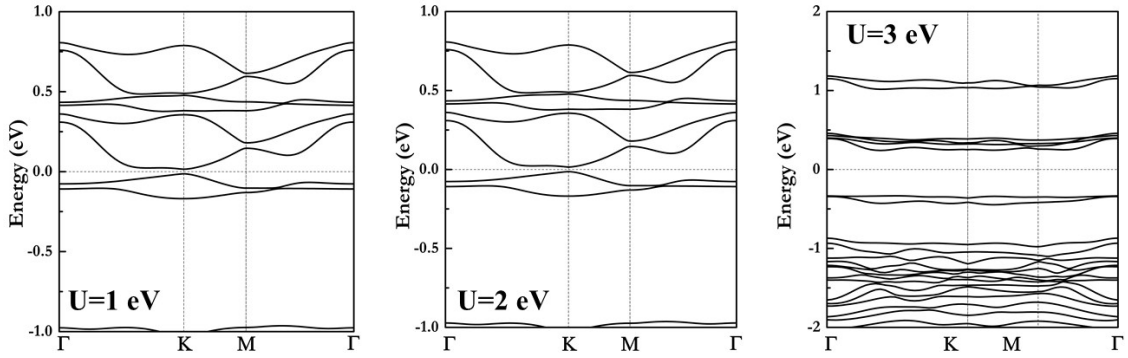

Figure S9. Band structures of $PdBr_3$ calculated by GGA +U with SOC.

Table S1. The relative energies between the FM and AFM states.

E(eV/f.u.)	FM	AFM-Neel	AFM-zigzia	AFM-stripy
VBr_3	0	0.221	0.123	0.075
$FeBr_3$	0	-0.791	-0.804	-0.780
$NiBr_3$	0	0.130	0.131	0.126
$PdBr_3$	0	0.119	0.127	0.122

Table S2. Summary of magnetic anisotropy energies (MAE) in μeV/metal and the easy axis (EA) for the VBr_3, $NiBr_3$ and $PdBr_3$ monolayer.

MAE (μeV/metal)	**$E_{[001]}$-$E_{[1-10]}$**	**$E_{[1-10]}$-$E_{[110]}$**	**EA**
VBr_3	300	150	[110]
$NiBr_3$	377	-50	[1-10]
$PdBr_3$	463	196	[110]