Supplemental material for publication

Magnetic and electronic properties of 2D TiX_3 (X = F, Cl, Br, I)

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Table S1. Calculated lattice constants (Å) of TiX_3 monolayers with different U-J values

U-J/eV	3	4	5	6
TiF_3	5.55	5.61	5.62	5.63
$TiCl_3$	6.29	6.33	6.35	6.38
$TiBr_3$	6.65	6.66	6.68	6.68
TiI_3	7.15	7.19	7.20	7.21

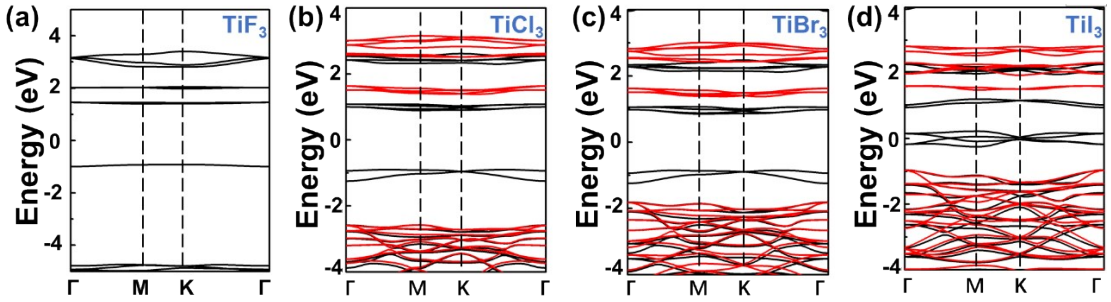

Fig. S1 Electronic band structures of (a) TiF_3, (b) $TiCl_3$, (c) $TiBr_3$ and (d) TiI_3 calculated with U-J = 3 eV from the DFT + U method. The Fermi level was set to 0 eV. Γ (0, 0, 0), M (1/2, 0, 0), and K (1/3, 1/3, 0) are highly symmetric points in reciprocal space. Red - spin down; black - spin up.

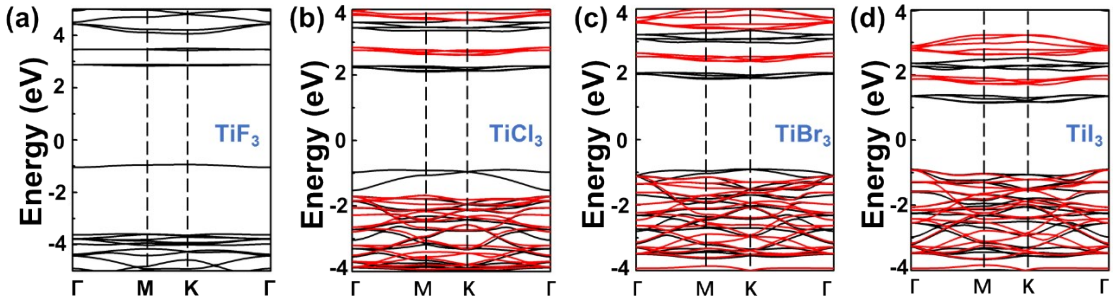

Fig. S2 Electronic band structures of (a) TiF_3, (b) $TiCl_3$, (c) $TiBr_3$ and (d) TiI_3 calculated with U-J = 5 eV from the DFT + U method. The Fermi level was set to 0 eV. Γ (0, 0, 0), M (1/2, 0, 0), and K (1/3, 1/3, 0) are highly symmetric points in reciprocal space. Red - spin down; black - spin up.

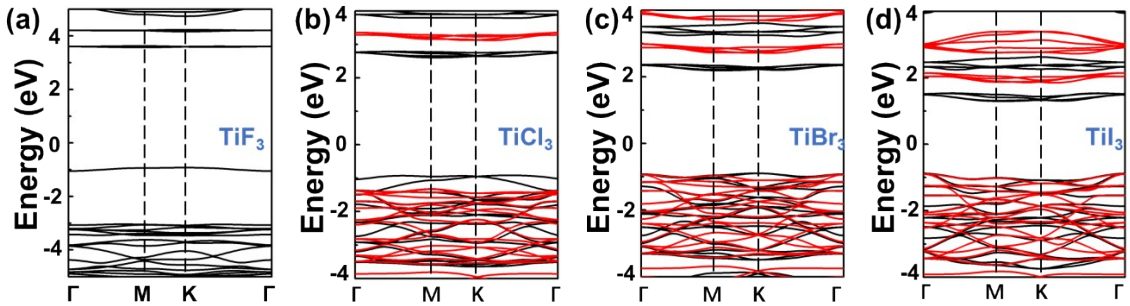

Fig. S3 Electronic band structures of (a) TiF_3, (b) $TiCl_3$, (c) $TiBr_3$ and (d) TiI_3 calculated with U-J = 6 eV from the DFT + U method. The Fermi level was set to 0 eV. Γ (0, 0, 0), M (1/2, 0, 0), and K (1/3, 1/3, 0) are highly symmetric points in reciprocal space. Red - spin down; black - spin up.

Table S2 Band gaps (eV) of TiX_3 monolayers with different U-J values

U-J/eV	3	4	5	6
TiF_3	2.32	3.04	3.77	4.49
$TiCl_3$	1.79	2.39	2.99	3.52
$TiBr_3$	1.70	2.27	2.76	3.09
TiI_3	0.02	1.91	2.05	2.18

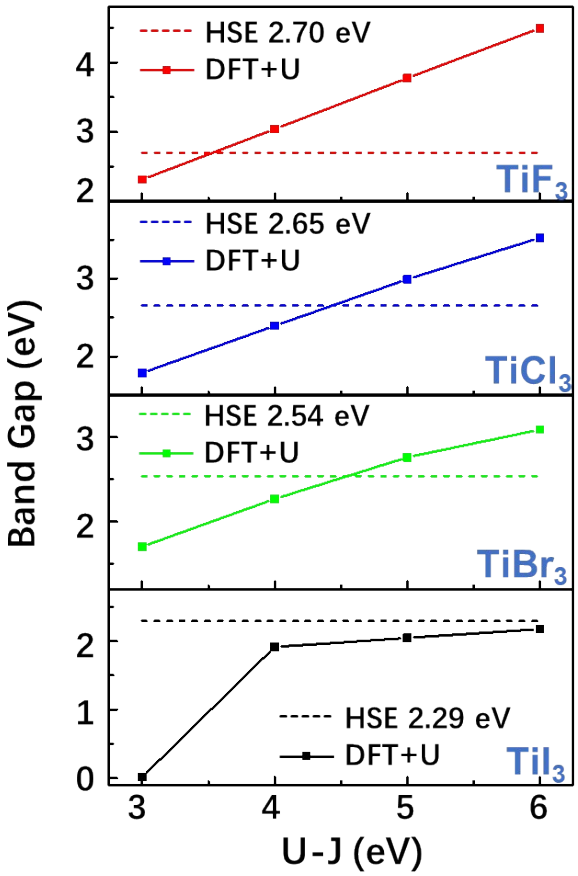

Fig. S4 Band gap of (a) TiF_3, (b) $TiCl_3$, (c) $TiBr_3$ and (d) TiI_3 as a function of U compared with the band gaps calculated with HSE06.

Tab. S3 Calculated total magnetic moments per unit cell (M_{tot}), local Magnetic moments of Ti (M_{Ti}) and Br/I (M_X) in monolayer $TiBr_3$ and TiI_3

	$TiBr_3$			TiI_3		
	FM	AFM-N	AFM-z	FM	AFM-N	AFM-z
M_{tot}(μb)	1.71	0	0	1.72	0	-0.02
M_{Ti}(μb)	0.98	-0.95/0.95	-0.97/0.97	1.04	-1.01/1.01	-1.02/1.02
M_X(μb)	-0.04	0	-0.04/0.04	-0.06	0	-0.05/0.05

Tab. S4 Exchange energies (E_{ex}) of TiX_3 monolayers (per TiX_3 formula meV/s.f.) with different U-J values

U-J/eV	3	4	5	6
TiF_3	-2.01	-3.01	-1.67	-1.28
$TiCl_3$	4.23	3.94	2.10	1.72
$TiBr_3$	3.88	27.54	27.39	27.56
TiI_3	3.56	26.24	25.68	26.01