Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Enriching the 2D transition metal borides via MB XMenes (M=Fe, Co, Ir): Strong correlation and magnetism

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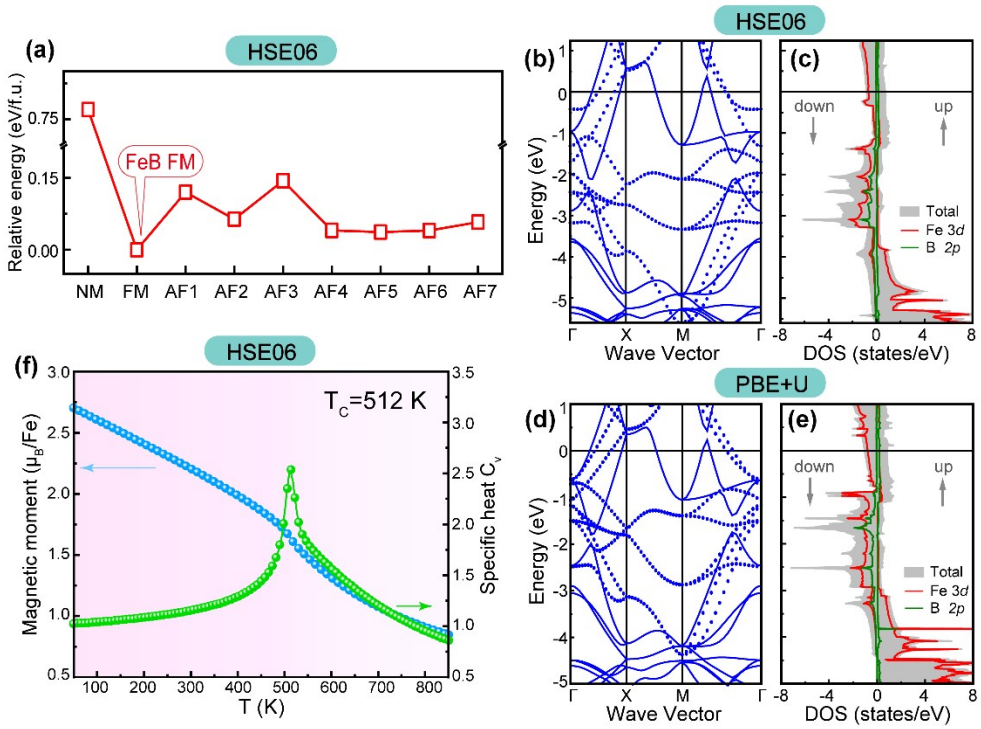

Fig. S1 (a) Relative energies (in eV/f.u.) of the non-magnetic and eight collinear magnetic FeB configurations obtained from the HSE06 functional. (b-e) Calculated band structure, total and projected density of states for FeB monolayer in its magnetic ground state by employing (b, c) HSE06 and (d, e) PBE+U function,

respectively. The blue solid and dotted line representing the spin-up and spin-down states. The Fermi level is set to zero. (f) The magnetic moment and specific heat C_v of FM-FeB XMene as a function of temperature calculated by HSE06 functional.

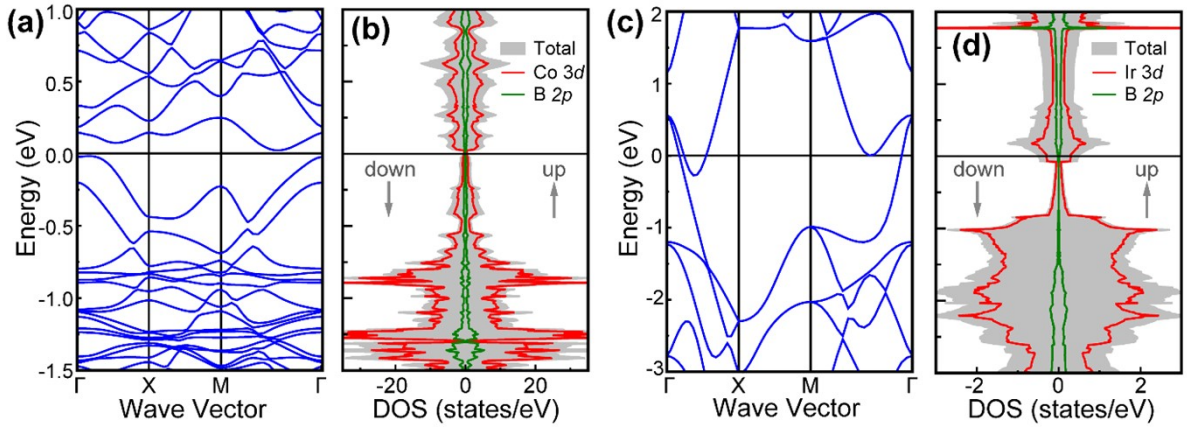

Fig. S2 Calculated band structure, total and projected density of states for (a, b) CoB and (c, d) IrB monolayers in their magnetic ground state (respectively AF4 and NM). The Fermi level is set to zero.

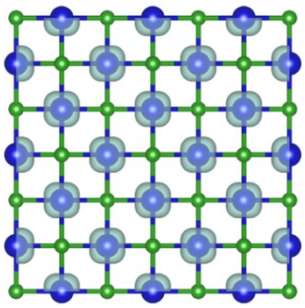

Fig. S3 The spatial distributions of spin densities with an isosurface of 0.03 e/Å^3 for the FM-FeB monolayer.

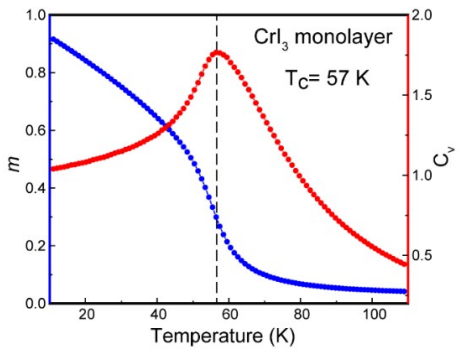

Fig. S4 The normalized magnetization and specific heat as a function of temperature for the CrI_3 monolayer.

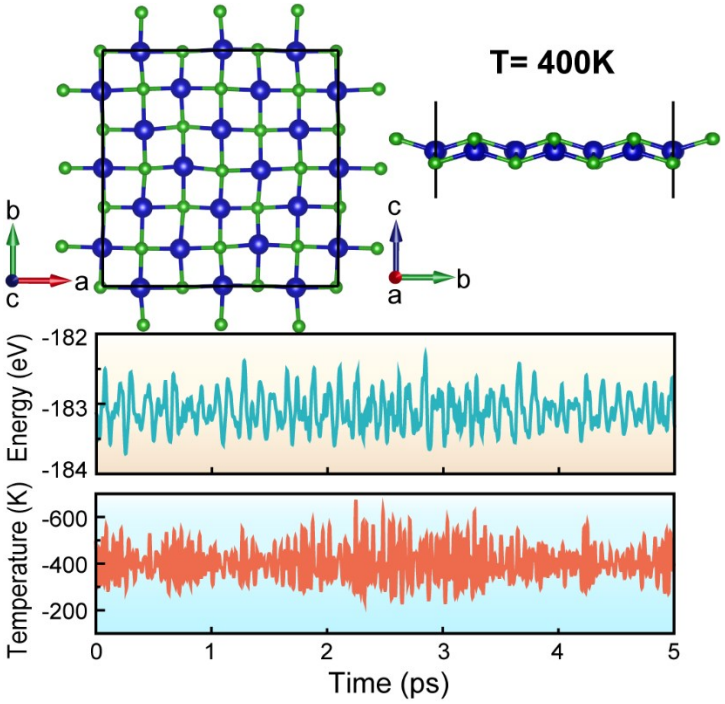

Fig. S5 The final structure and the evolution of energy (eV) and corresponding temperature (K) during the 5 *ps* AIMD at 400 K for the 2D FeB monolayer with FM configuration.

Table S1 Calculated lattice constants *a* (Å), M-B bond lengths *l* (Å), layer thickness *h* (Å), and the magnetic moment projected on Fe atom M_{Fe} (μ_B/Fe) of FeB monolayer under PBE+U and HSE06 functionals.

	U_{eff} = 1	U_{eff} = 2	U_{eff} = 3	U_{eff} = 3.96	U_{eff} = 5	HSE06
a	3.71	3.76	3.74	**3.86**	4.04	**3.82**
l	1.93	1.92	1.94	**2.02**	2.02	**2.00**
h	1.14	0.97	1.11	**1.20**	0	**1.19**
M_{Fe}	1.40	1.51	1.59	**2.42**	2.99	**2.31**