

Supporting Information for

TMB₁₂: A Newly Designed 2D Transition-Metal Borides for Spintronics and Electrochemical Catalyst Applications

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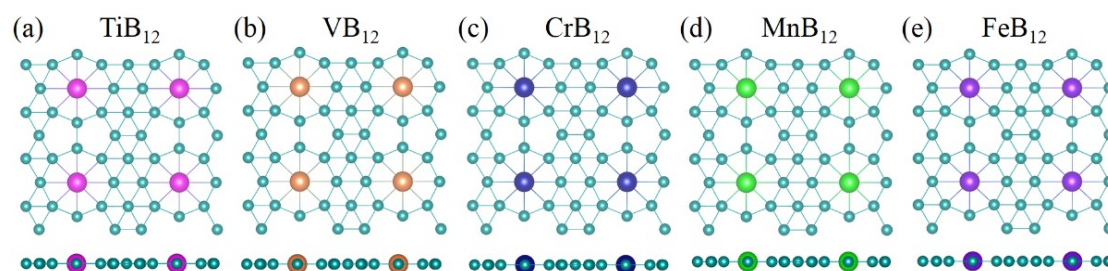


Fig. S1 The optimized structures of TMB₁₂(TM=Ti, V, Cr, Mn, and Fe) monolayer. The magenta, orange, dark-blue, green, purple and teal balls represent Ti, V, Cr, Mn, Fe and B atoms, respectively.

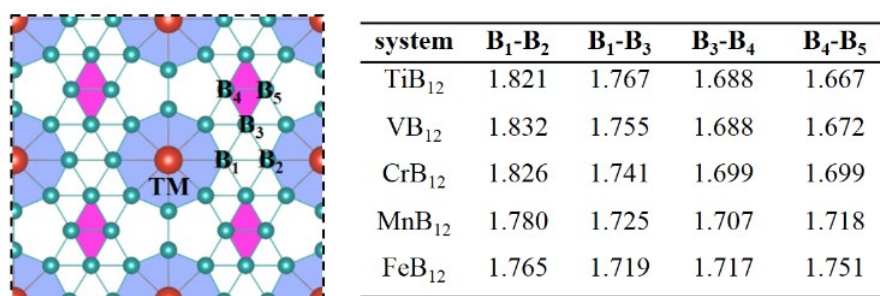


Fig. S2 The lengths (Å) of party of the B-B bonds in the TMB₁₂ structure.

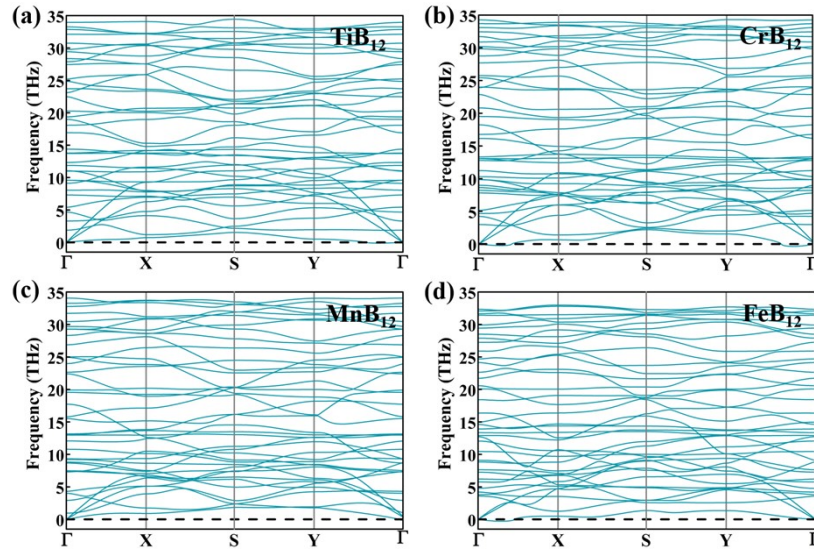


Fig. S3 The phonon spectrum of (a) TiB_{12} ; (b) CrB_{12} ; (c) MnB_{12} ; and (d) FeB_{12} monolayer.

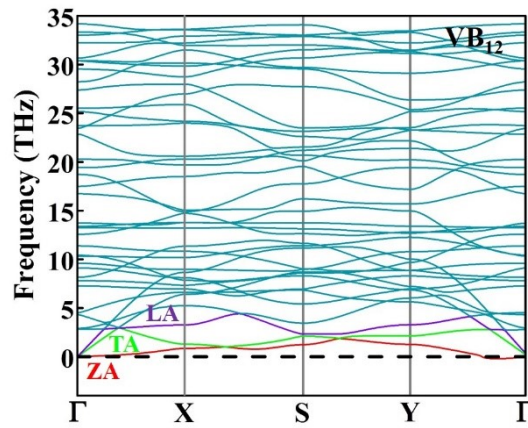


Fig. S4 The phonon spectrum of the VB_{12} monolayer.

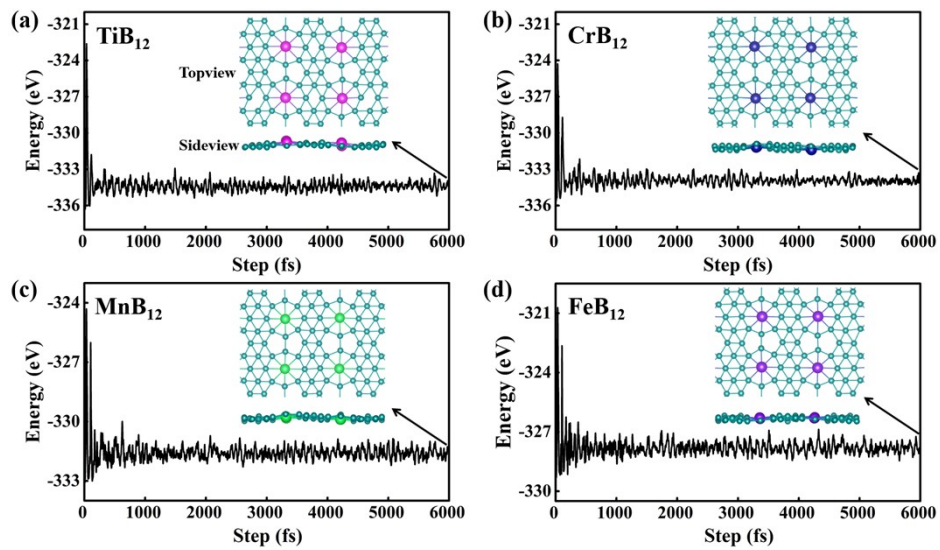


Fig. S5 AIMD simulation of (a) TiB_{12} ; (b) CrB_{12} ; (c) MnB_{12} ; and (d) FeB_{12} monolayer at 300 K for 6 ps.

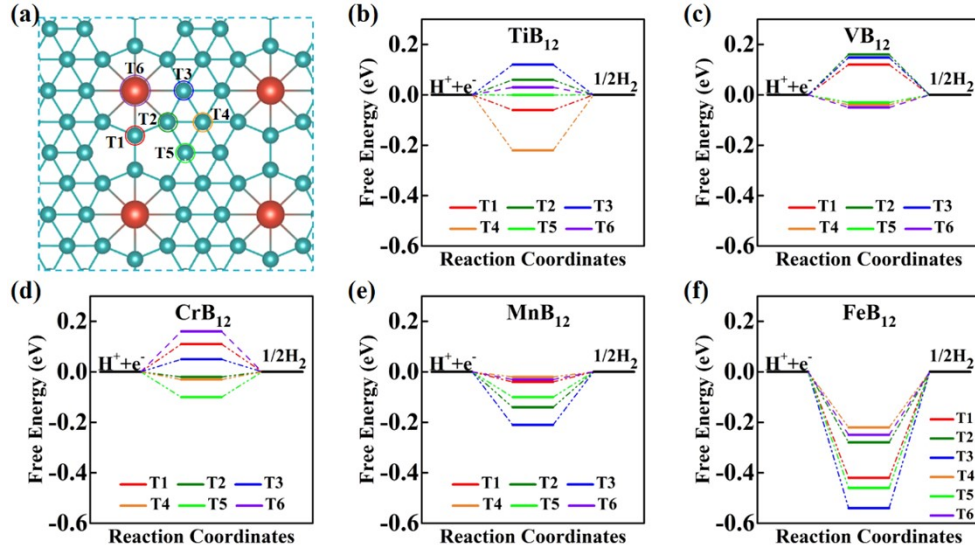


Fig. S6 (a) Illustration of six different hydrogen adsorption sites on TMB_{12} monolayer. (b-f) The Gibbs free energy of six hydrogen adsorption sites for TMB_{12} (TM = Ti, V, Cr, Mn and Fe) monolayer.

Table S1 Calculated elastic constants C (in kbar) of TMB_{12} .

system	C_{11}	C_{22}	C_{12}	C_{66}
TiB_{12}	1070.2	1335.0	291.40	501.8
VB_{12}	1122.8	1306.6	273.1	447.0
CrB_{12}	984.3	1268.8	213.3	477.0
MnB_{12}	981.1	1233.3	234.6	467.1
FeB_{12}	398.9	1190.8	119.9	438.1

Table S2. Calculated MAEs along different magnetic directions, the easy axis, and magnetic exchange parameters (J_1 and J_2) for TMB_{12} (TM = V, Cr, Mn, Fe).

system	100 (eV)	010 (eV)	001 (eV)	MAE (μeV)	Easy axis	J_1 (meV)	J_2 (meV)
VB_{12}	-80.749029	-80.749101	-80.749044	72	(010)	25.0	63.7
CrB_{12}	-80.957244	-80.957053	-80.957476	423	(001)	27.2	22.0
MnB_{12}	-81.129102	-81.129002	-81.129625	623	(001)	10.4	-27.1
FeB_{12}	-80.157135	-80.157092	-80.157290	198	(001)	-7.83	-14.4