Supplementary materials for

First-principles Prediction of Two-dimensional MnOX (X=Cl, Br) Monolayers: The Half-metallic Multiferroics with Magnetoelastic Coupling

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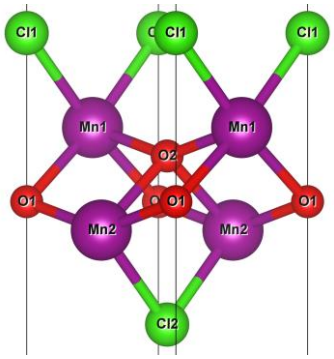

Fig. S1. The geometry structure of the MnOCl monolayer along the 110 axis.

Table S1. The structure parameters of MnOX monolayers. The lattice constants (Å), bond lengths (Å) and bond angles (degree) based on PBE functional.

	Lattice constants(Å)	Bond lengths (Å)		Bond angles(degree)	
MnOCl	a = 3.34 b = 3.78	Mn1-O1	2.13	∠Mn1-O1-Mn2	99.3
		Mn1-O2	1.96	∠Mn2-O2-Mn2	103.0
		Mn1-Cl1	2.38	∠Mn1-Cl1-Mn1	89.2
MnOBr	a = 3.42 b = 3.83	Mn1-O1	2.12	∠Mn1-O1-Mn2	98.4
		Mn1-O2	1.98	∠Mn2-O2-Mn2	107.7
		Mn1-Br1	2.53	∠Mn1-Br1-Mn1	84.8

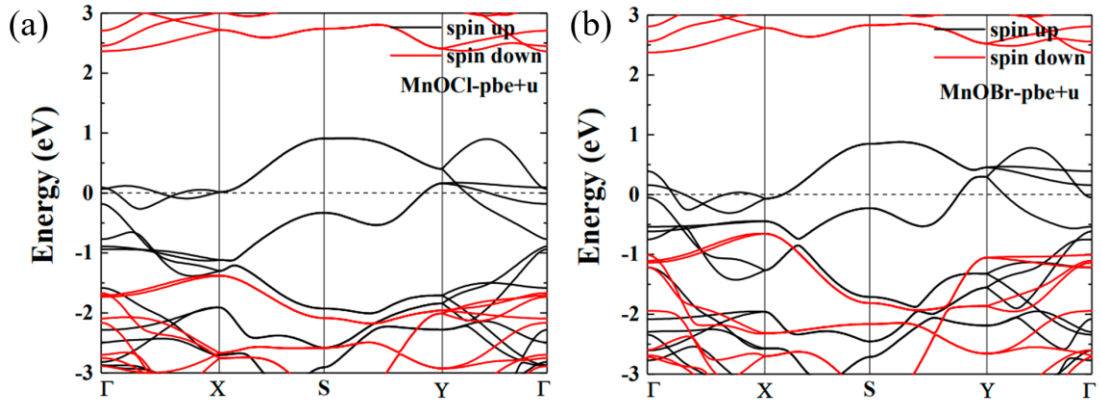

Fig. S2. Band structures of monolayer MnOCl and MnOBr based on PBE+U.

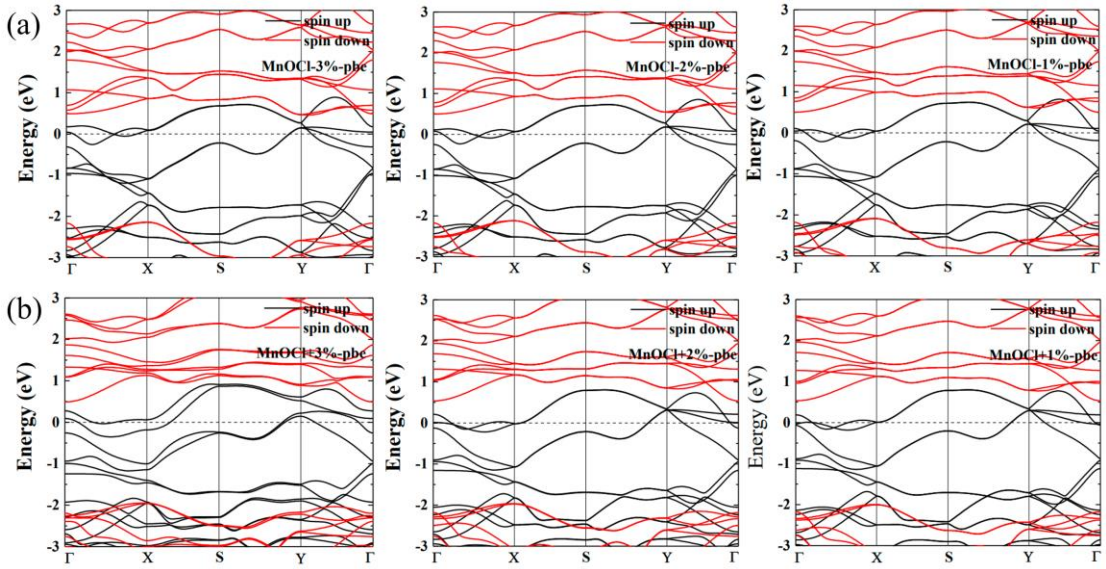

Fig. S3. Band structures of Monolayer MnOCl under biaxial (a) compressive strain and (b) tensile strain.

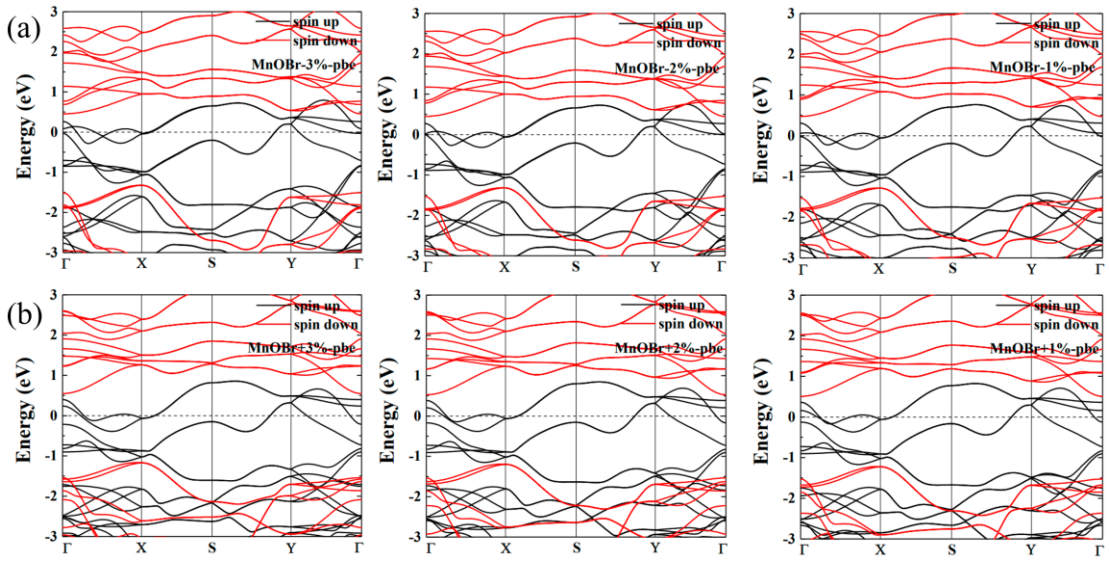

Fig. S4. Band structures of Monolayer MnOBr under biaxial (a) compressive strain and (b) tensile strain.

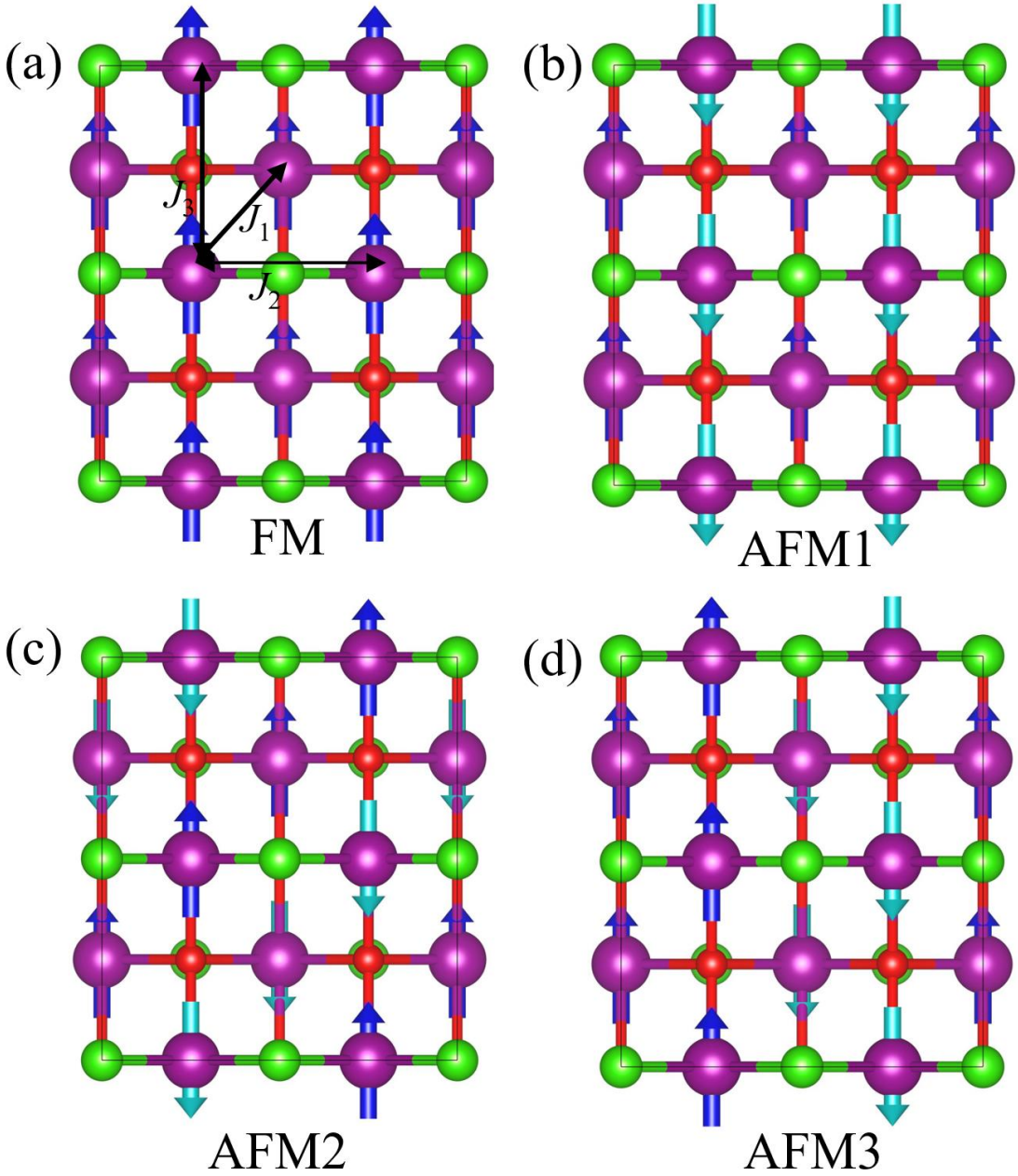

Fig. S5. Possible four magnetic configurations: (a) FM, (b) AFM1, (c) AFM3, (d) AFM4. J_1, J_2 and J_3 present the magnetic exchange interaction between the first-nearest, second-nearest and third nearest Mn atom, respectively.

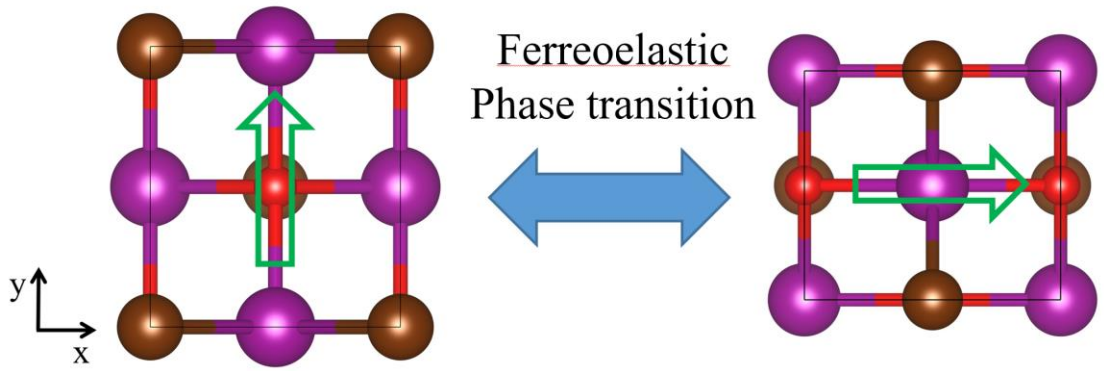

Fig. S6. Magnetoelastic coupling in MnOBr monolayer. Blue arrows present the net magnetic moment directions.

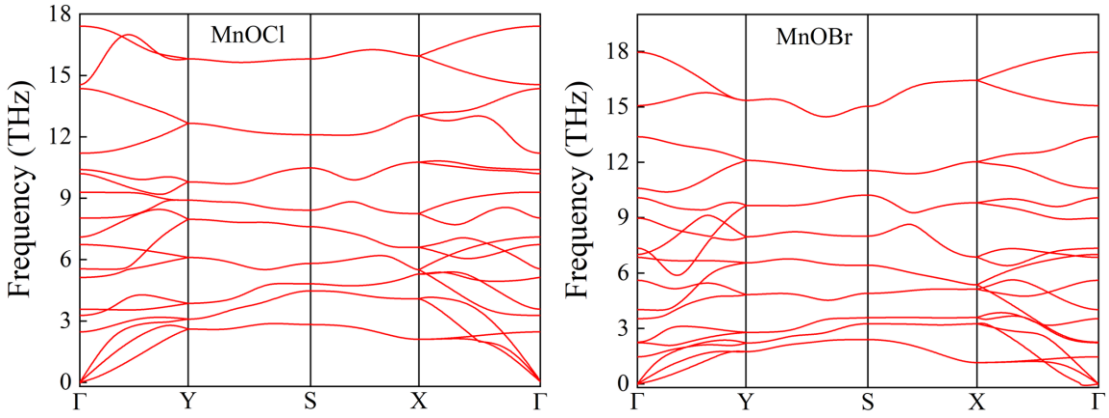

Fig. S7. Phonon dispersion spectrums of 2D MnOX monolayers.

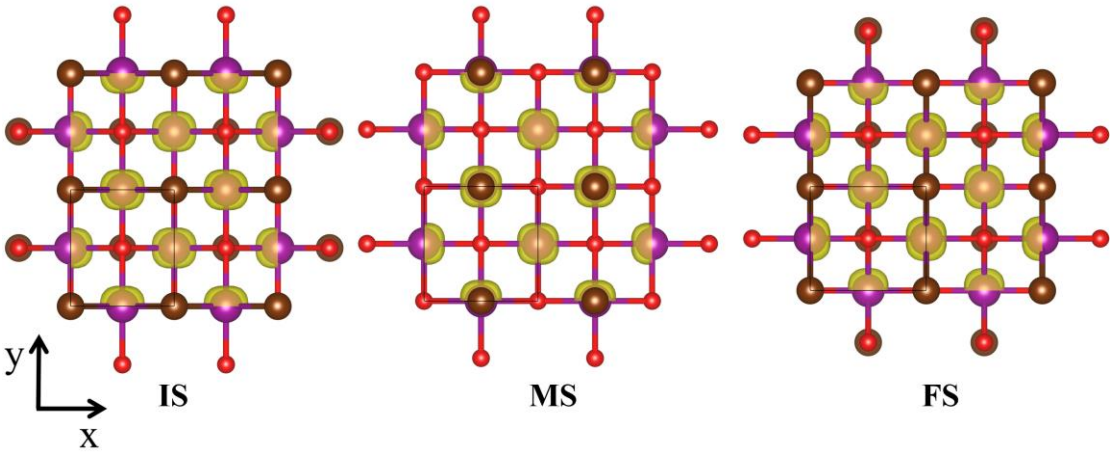

Fig S8. Spin charge densities of the IS, MS and FS states in the MnOBr monolayer (isosurface value of 0.07 e/Bohr^3).

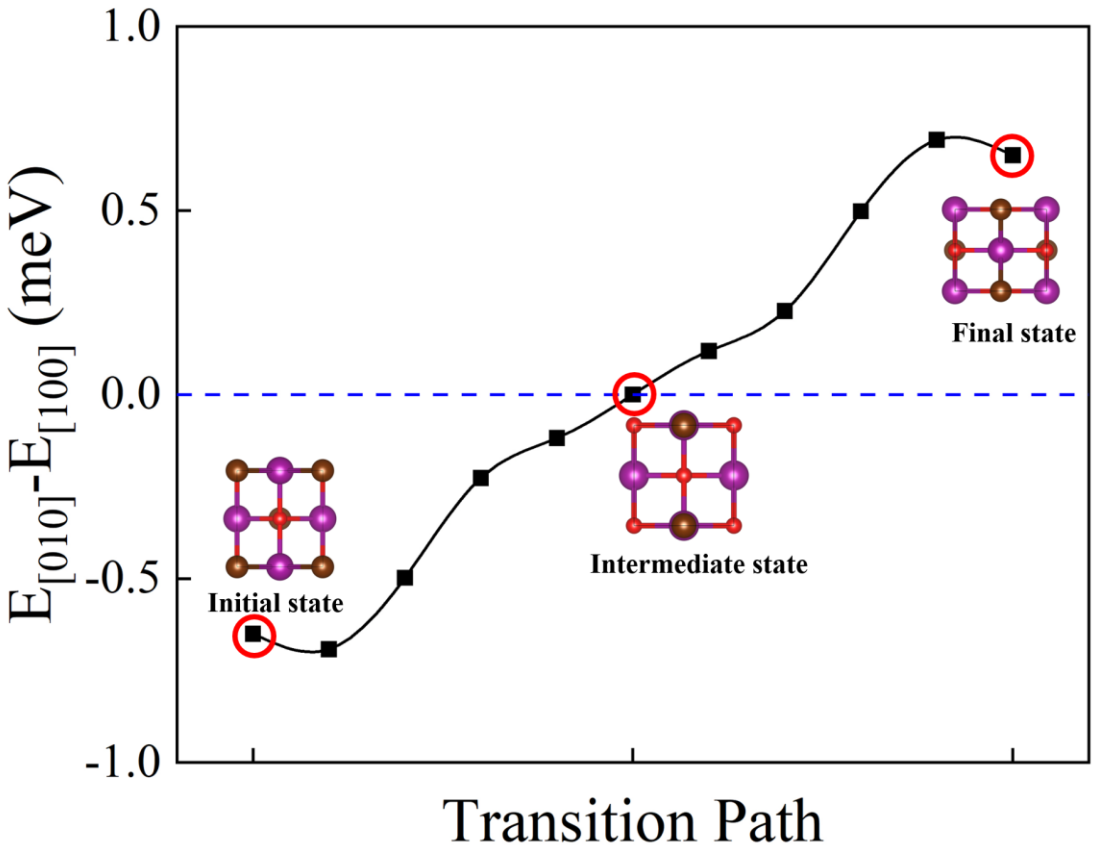

Fig S9. the changes of the MAE in the ferroelastic phase transition of the MnOBr monolayer.