

Predicting Intrinsic Antiferromagnetic and Ferroelastic MnF₄ monolayer with Controllable Magnetization

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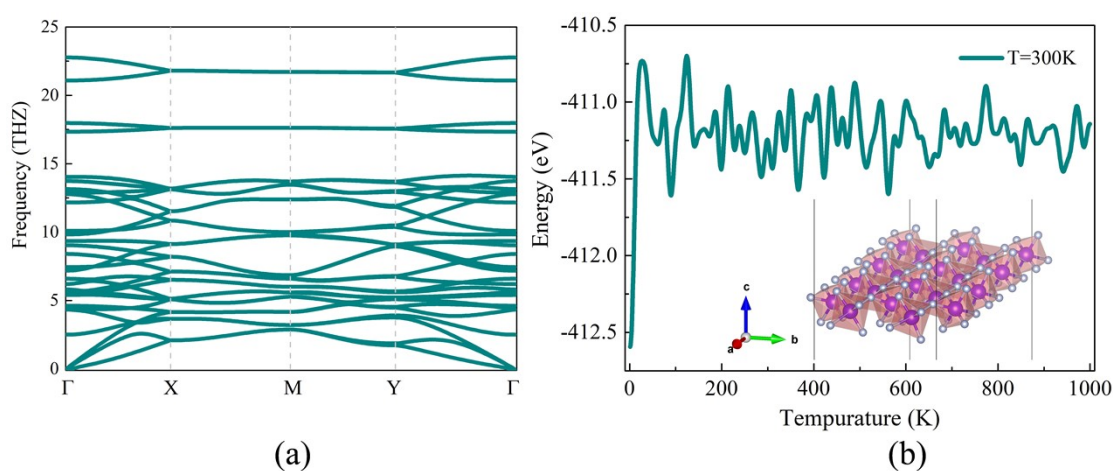


Figure S1 (a) The phonon spectra of the MnF₄ monolayer. (b) The evolution of energy over time at T=300 K from molecular dynamics simulations of MnF₄ monolayer.

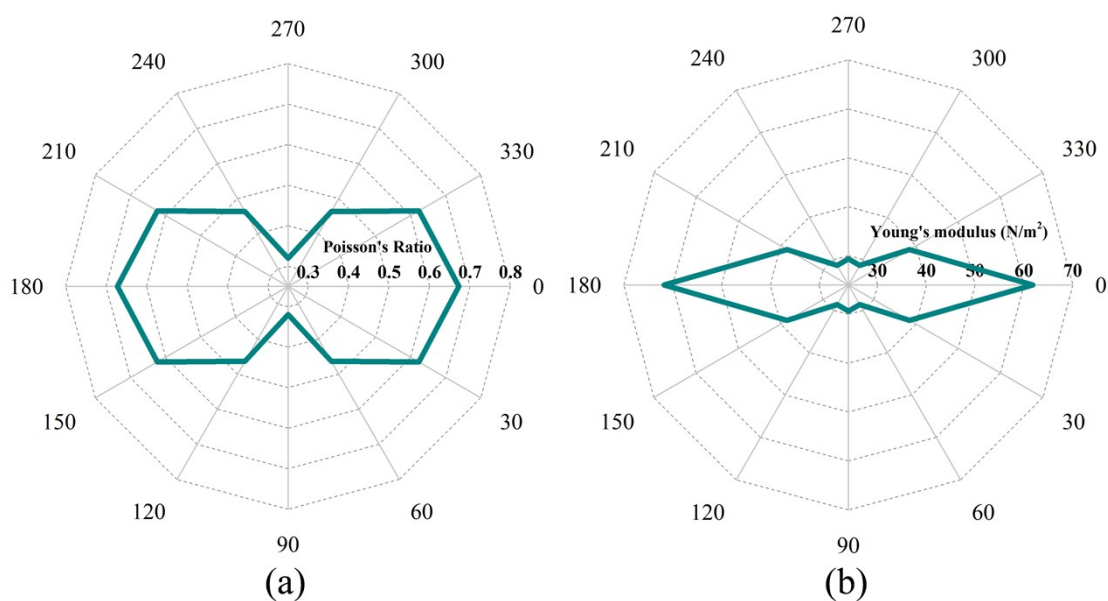


Figure S2 The angular dependence of (a) Young's modulus and (b) Poisson's ratio of the MnF₄ monolayer. The zero degree corresponds to *a*-axis.

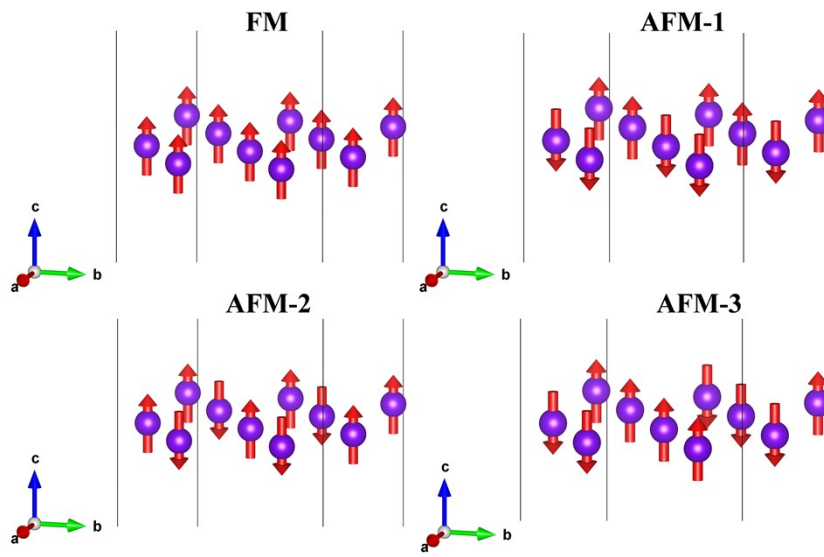


Figure S3 Four magnetic configurations of MnF₄ monolayer. The arrows along *c*-axis and *-c*-axis represent spin up and spin down moments respectively.

Table S1 The calculated elastic constants (N/m) of the MnF₄ monolayer.

System	C_{11}	C_{12}	C_{22}	C_{66}
MnF ₄ monolayer	78.626	25.096	37.337	9.957

Table S2 The relative energy ($E_{\text{FM}}-E_{\text{AFM}i=1-3}$) of four different configurations of MnF_4 monolayer as a function of carrier density.

Carrier density	FM (meV)	AFM1(meV)	AFM2(meV)	AFM3(meV)
-0.20e	0.000	-6.808	-22.188	-6.908
-0.15e	0.000	-7.302	-21.297	-7.9.00
-0.10e	0.000	-0.002	-8.900	-0.0152
-0.05e	0.000	13.330	9.29432	11.595
0	0.000	25.550	26.341	35.800
0.05e	0.000	25.207	17.740	22.105
0.10e	0.000	-16.786	-23.308	-17.887
0.15e	0.000	-55.737	-65.228	-56.838
0.20e	0.000	-105.708	-118.164	-106.903

Table S3 The relative energy ($E_{\text{FM}}-E_{\text{AFM}i=1-3}$) of four different configurations of MnF_4 monolayer as a function of biaxial strains.

Strain	FM	AFM1	AFM2	AFM3
-4%	0.000	-752.450	-747.718	-752.554
-3%	0.000	-371.088	-367.578	-372.345
-2%	0.000	-97.685	-96.102	-97.886
-1%	0.000	182.796	179.453	182.555
0%	0.000	213.717	210.526	213.656
+1%	0.000	190.772	184.790	190.972
+2%	0.000	126.498	122.143	126.500
+3%	0.000	5.05845	1.57518	5.05491
+4%	0.000	-229.495	-233.188	-229.499