Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information

Prediction of two-dimensional antiferromagnetic ferroelasticity in AgF_2 monolayer

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Table S1. The band gaps of SL AgF_2 using different methods.

Method	PBE	HSE06	PBE+U (3eV)
Band gap (eV)	0.31	2.87	1.23

Table S2. The cleavage energy with different methods.

Method	PBE+D3 Vdw	PBE+D2 Vdw	LDA	LDA+D3 Vdw
c (Å)	5.73	5.56	5.45	5.36
cleavage energy ($eV/Å^2$)	36.2	42.8	41.3	52.5

*Vdw denotes Van der Waals correction.

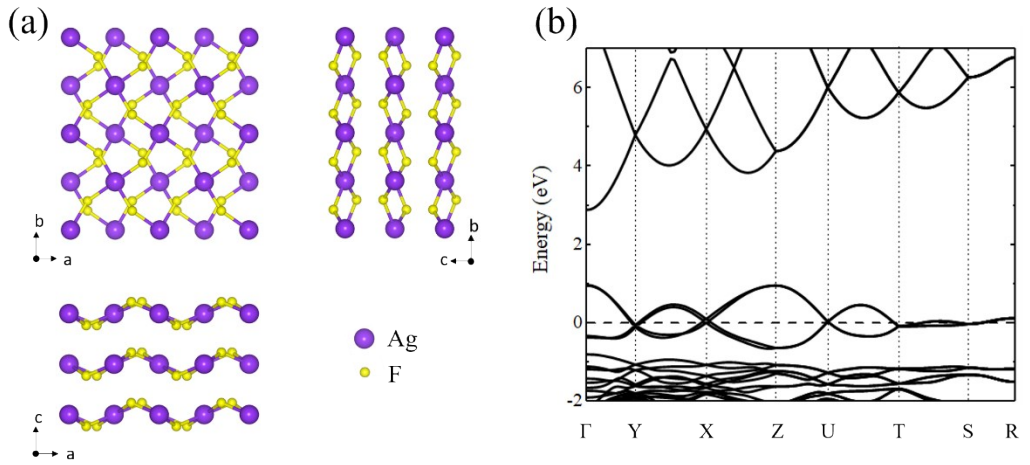

Fig. S1. (a) Crystal structures of bulk AgF_2 from top and side views. (b) The band structures of bulk AgF_2.

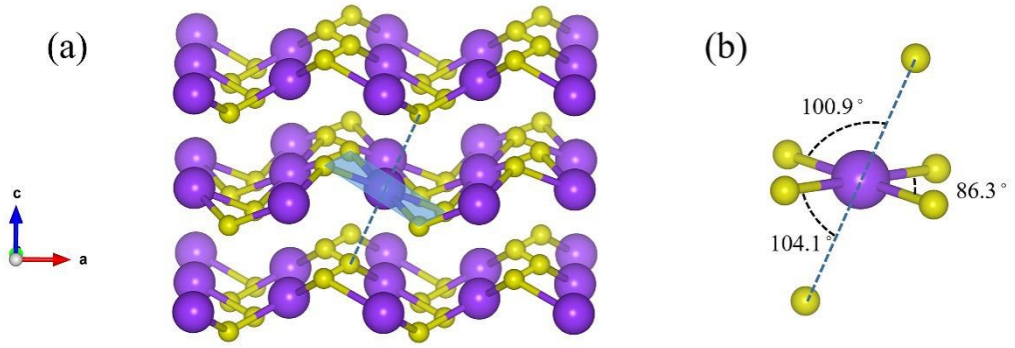

Fig. S2. The Jahn-Teller effect in bulk AgF_2.

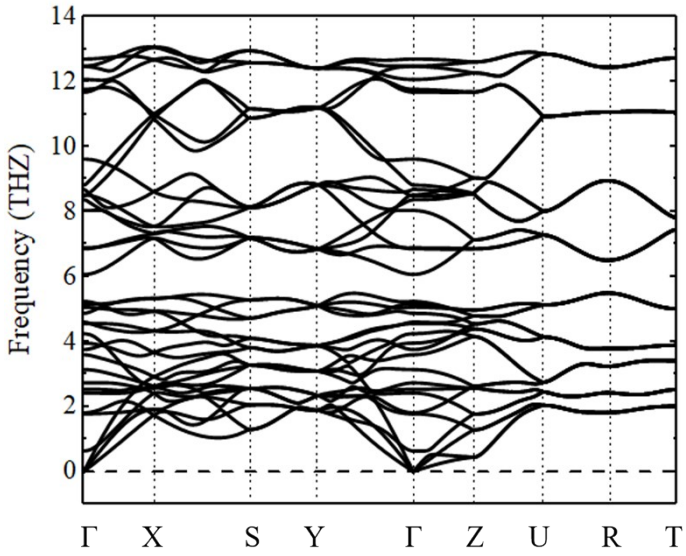

Fig. S3. The phonon bands of bulk AgF_2.

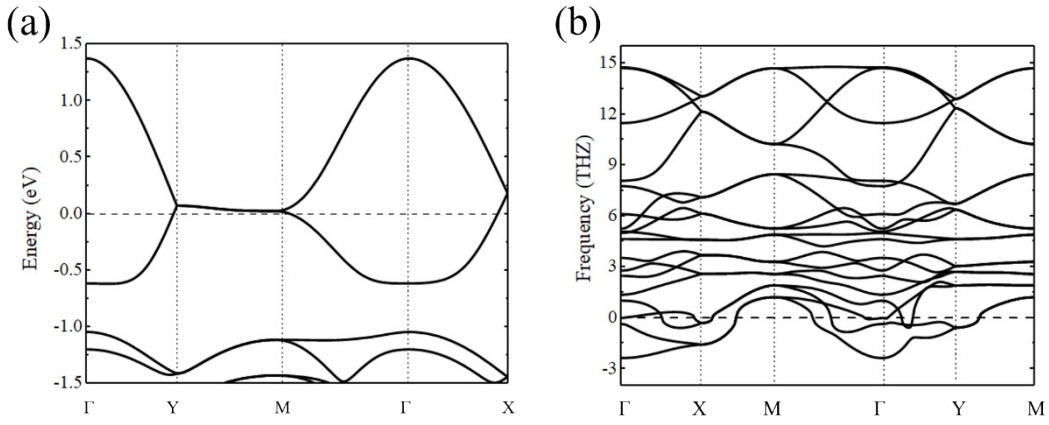

Fig. S4. (a) The band structures and (b) the phonon bands of SL AgF_2 with lattice parameters of bulk AgF_2.

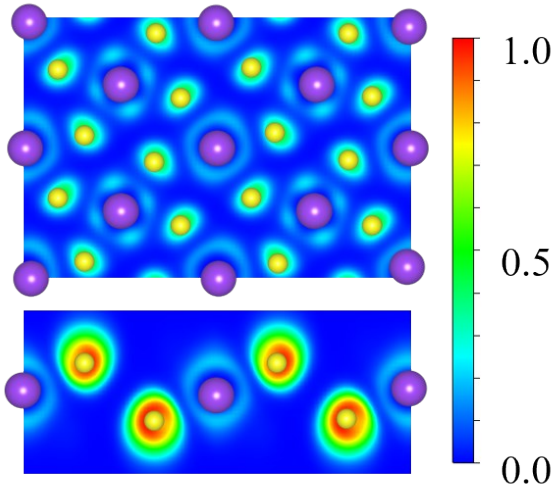

Fig. S5. Electronic localization function (ELF) for AgF_2 monolayer.

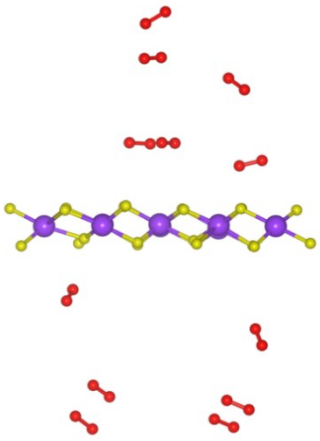

Fig. S6. The MD of AgF_2 monolayer with oxygen (2 ps at 300 K).