Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Magnetic Order-dependent phonon properties in 2D Magnet CrI_3

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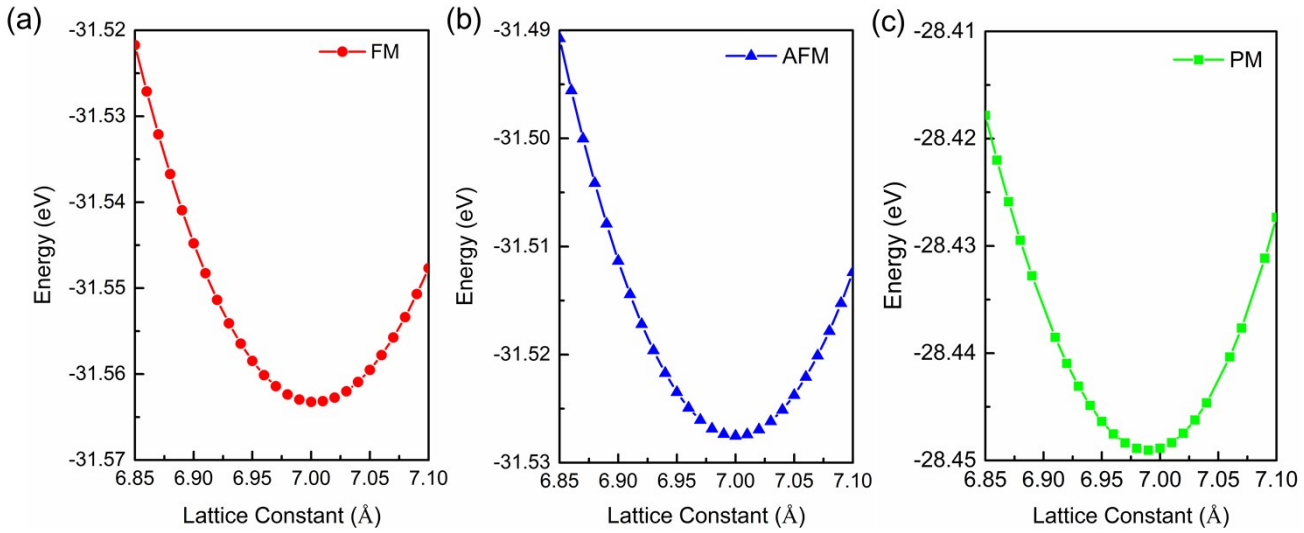


Figure S1. Optimization of lattice constant of CrI_3 monolayer with FM (a), AFM (b), and PM (c) phases.

Table S1. Frequencies and Grüneisen constants of 21 optical modes at Γ point.

FM			AFM			PM		
mode	Frequency (THz)	γ	mode	Frequency (THz)	γ	mode	Frequency (THz)	γ
1,2	1.371	0.943	1,2	1.364	0.767	1,2	1.275	-0.535
3	1.535	1.894	3	1.544	1.838	3	1.607	1.179
4	2.017	1.624	4	2.0187	1.573	4	2.175	1.536
5,6	2.119	0.644	5,6	2.200	0.706	5,6	2.537	0.580
7	2.521	0.856	7	2.554	0.843	7,8	2.810	-1.836
8,9	2.876	0.672	8,9	2.810	-0.242	9	2.862	0.0903
10,11	2.963	0.165	10,11	2.970	0.318	10,11	3.098	0.842
12,13	3.076	0.867	12,13	3.118	1.096	12,13	3.340	-0.117
14	3.569	0.540	14	3.494	0.173	14	3.781	-0.311
15	3.591	0.622	15	3.609	0.851	15	4.118	0.794
16	5.855	0.720	16	5.967	0.484	16	4.729	2.253
17,18	6.151	0.825	17,18	6.256	0.756	17,18	6.215	-0.526
19,20	6.598	0.681	19,20	6.557	0.352	19,20	6.412	0.500
21	7.314	0.675	21	7.247	0.664	21	6.788	0.082

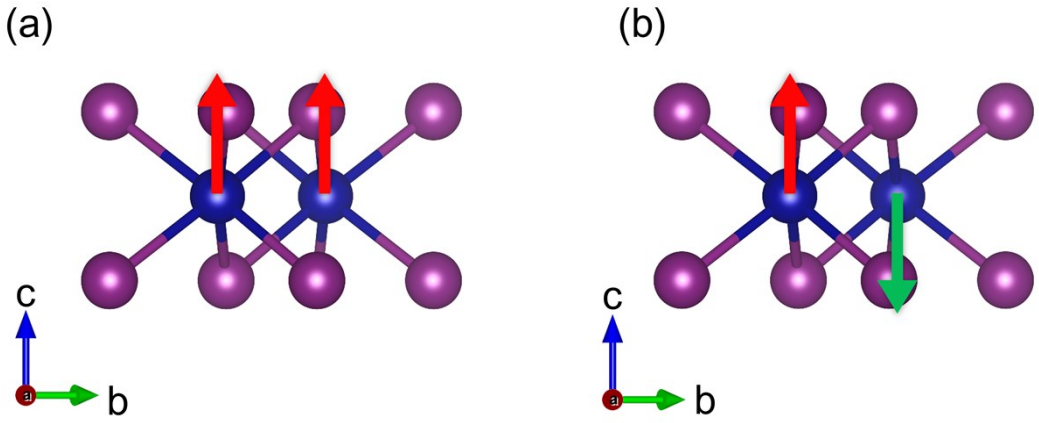
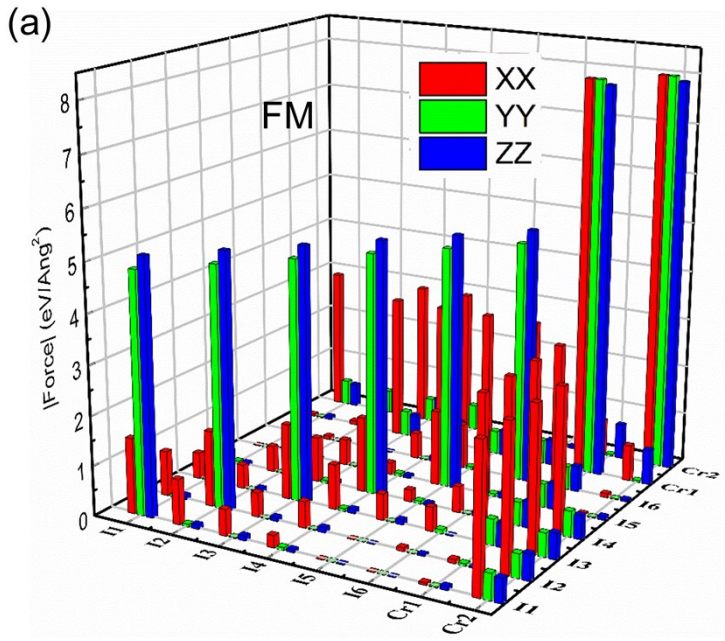


Figure S2. The ferromagnetic (FM) (a) and antiferromagnetic (AFM) (b) configurations for CrI_3 monolayer. The spin up and spin down are represented by the red and green arrows, respectively.



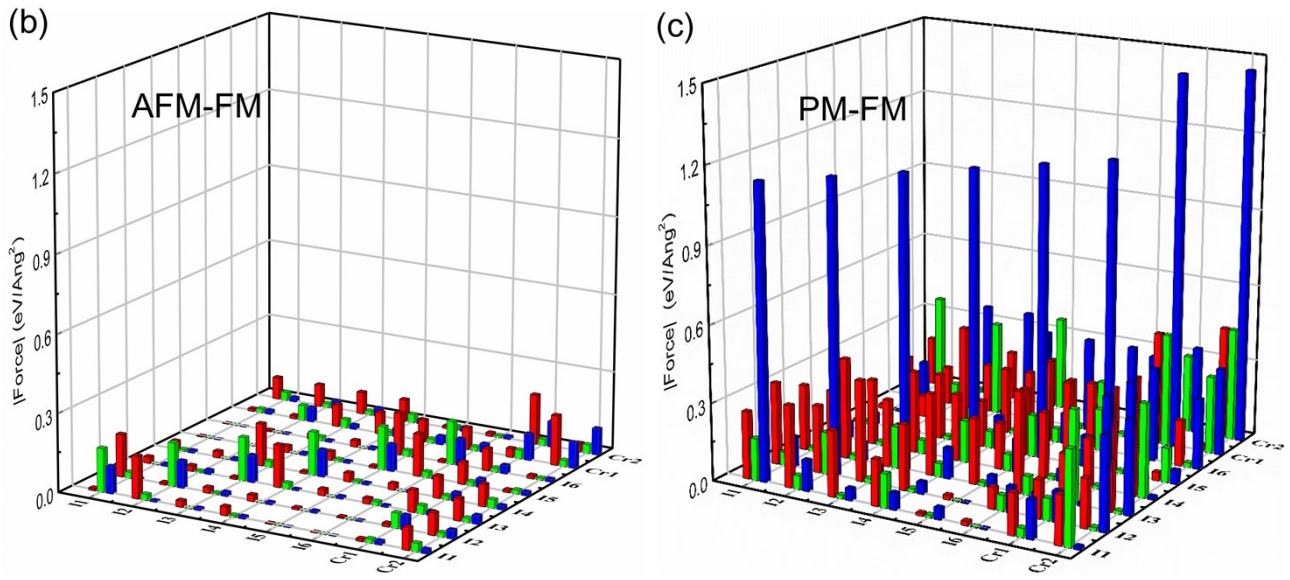


Figure S3. Interatomic force constants for CrI_3 with FM phase (a), the differences between the interatomic force constants of AFM and FM (AFM-FM) phases (b) and between PM and FM (PM-FM) phases (c).

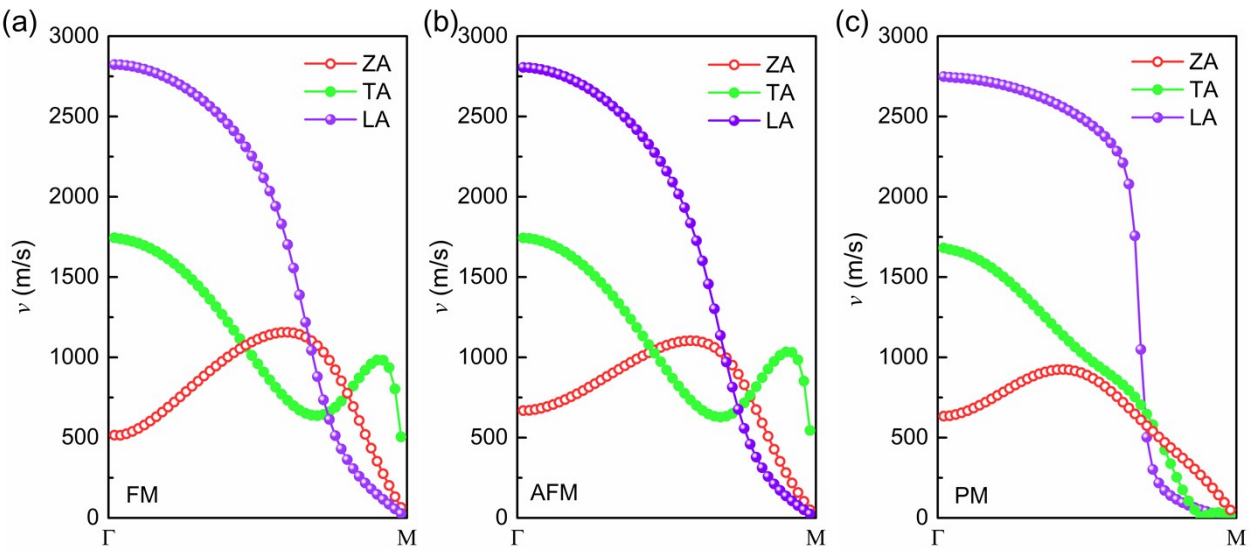


Figure S4. Group velocities of longitudinal acoustic (LA), transverse acoustic (TA) and out-of-plane acoustic (ZA) branches for CrI_3 monolayer with FM (a), AFM (b) and PM (c) configurations.

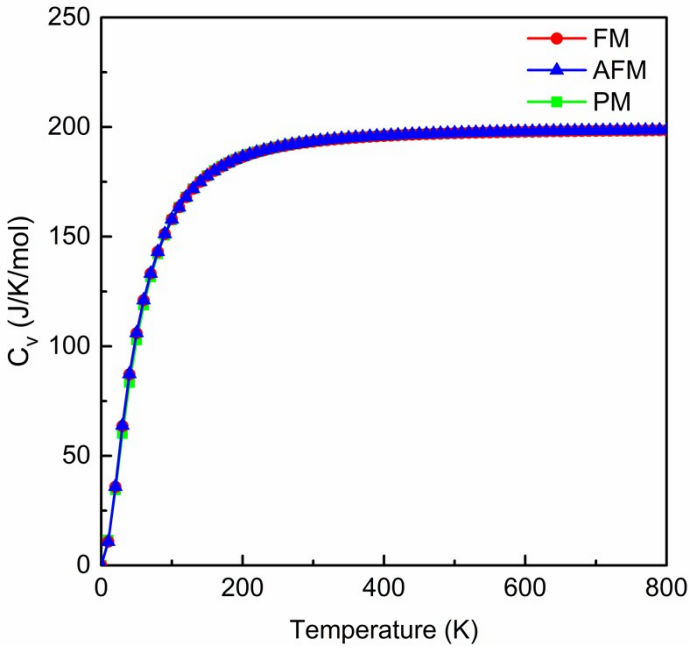


Figure S5. Specific heat capacity of CrI_3 monolayer as a function of temperature for FM, AFM and PM phases, respectively.

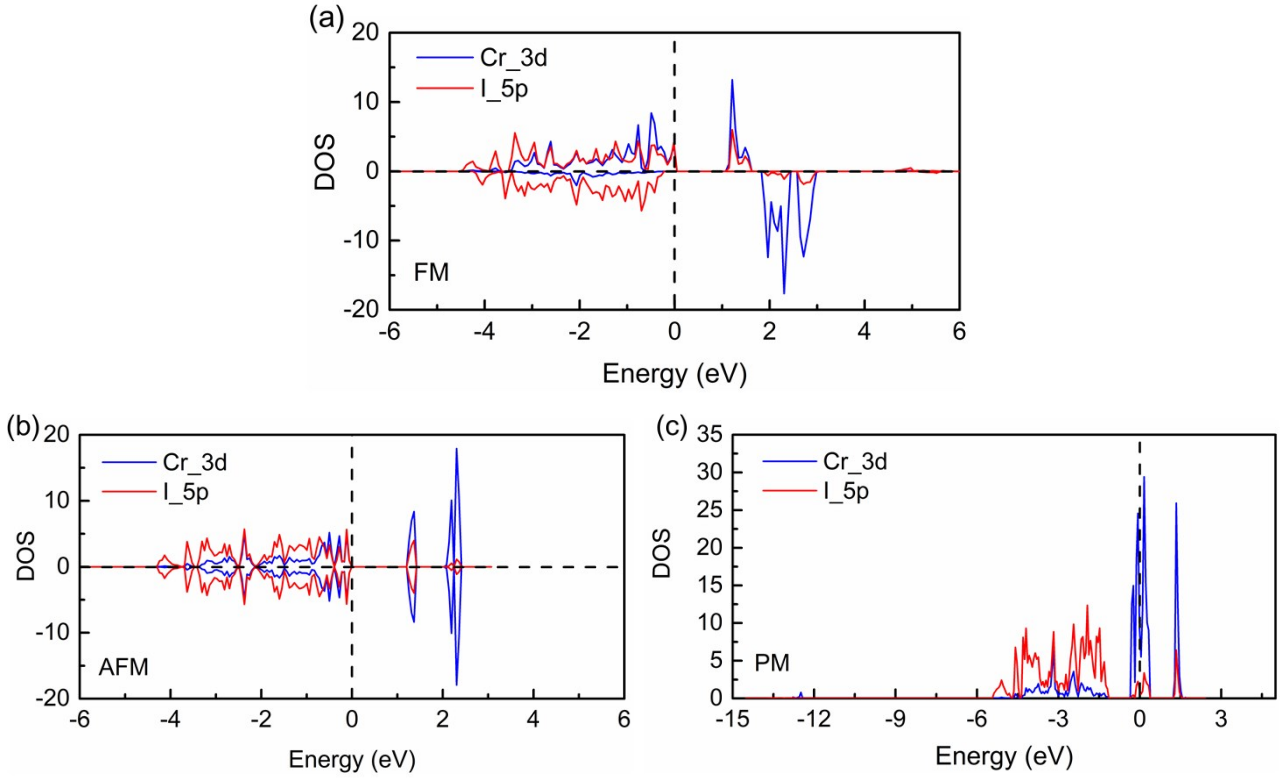


Figure S6. Electron density of states (DOS) of CrI_3 monolayer with FM (a), AFM (b), and PM (c) phases.

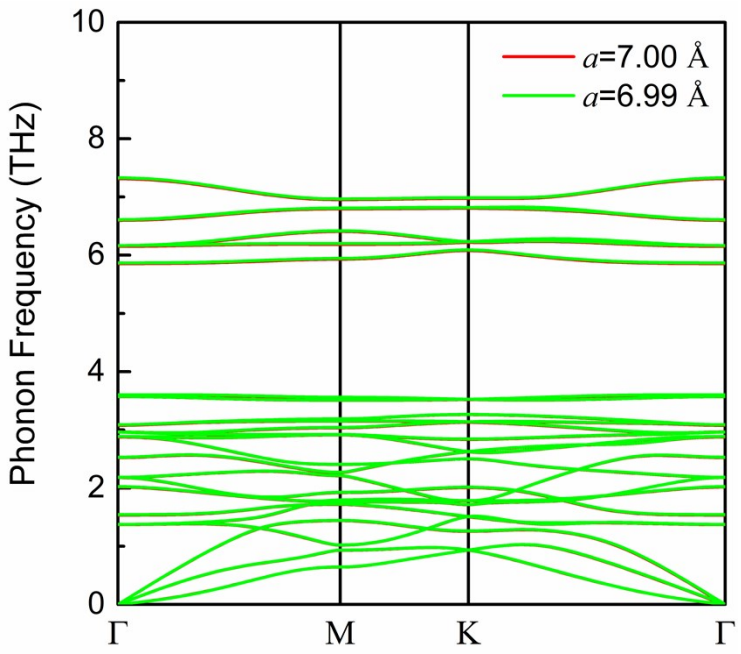


Figure S7. Phonon dispersion for FM-CrI_3 when lattice constant *a* is 7.00 and 6.99 Å, respectively.