supplementary material

Enhancement of Curie temperature under built-in electric field in Multi-functional Janus vanadium dichalcogenides

Shilei Ji(季石磊), Hong Wu(武红), Shuang Zhou(周双), Wei Niu(钮伟), Lujun Wei(魏陆军), Xing'ao Li(李兴鳌)[**], *Feng Li(李峰)*[**], *Yong Pu(普勇)*[**]

[1]*New Energy Technology Engineering Laboratory of Jiangsu Provence & School of Science, Nanjing University of Posts and Telecommunications (NJUPT), Nanjing 210023, China*

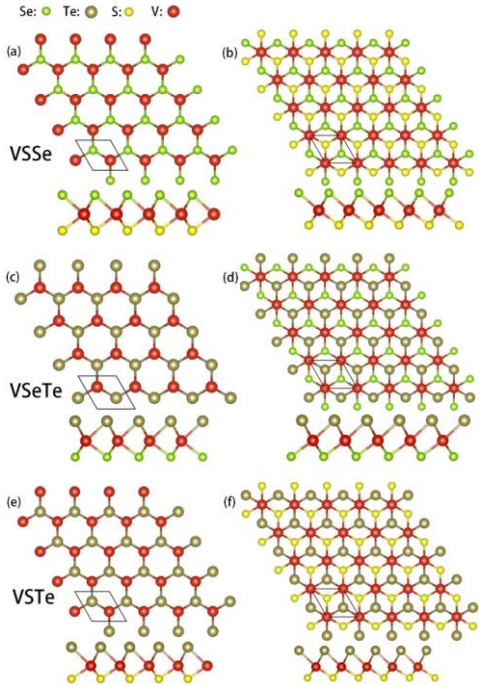

Fig. S1. The atomic structures of the 2H- (a) VSSe, (c) VSeTe, (e) VSTe and 1T- (b) VSSe, (d) VSeTe, (f) VSTe monolayers. The hexagonal primitive cells are labeled in dark solid lines. The red, yellow, green and brown balls are V, S, Se and Te atoms, respectively.

Table S1. The lattice constant, bond length, bond angle of the Janus VXX' monolayers.

	Lattice (Å)	V– S (Å)	V– Se (Å)	V– Te (Å)	V– S– V (deg)	V– Se– V (deg)	V– Te– V (deg)
2H-VS_2	3.17	2.36	—	—	84.34	—	—
2H-VSe_2	3.33	—	2.50	—	—	83.52	—
2H-VTe_2	3.57	—	—	2.72	—	—	82.14
2H-VSSe	3.25	2.35	2.51	—	87.26	80.69	—
2H-VSeTe	3.45	—	2.50	2.72	—	87.43	78.86
2H-VSTe	3.37	2.35	—	2.71	91.62	—	76.75
1T-VS_2	3.18	2.35	—	—	84.79	—	—
1T-VSe_2	3.34	—	2.49	—	—	83.99	—
1T-VTe_2	3.56	—	—	2.71	—	—	81.86
1T-VSSe	3.27	2.35	2.50	—	88.21	81.39	—
1T-VSeTe	3.46	—	2.48	2.72	—	88.14	78.96
1T-VSTe	3.41	2.34	—	2.73	93.36	—	77.07

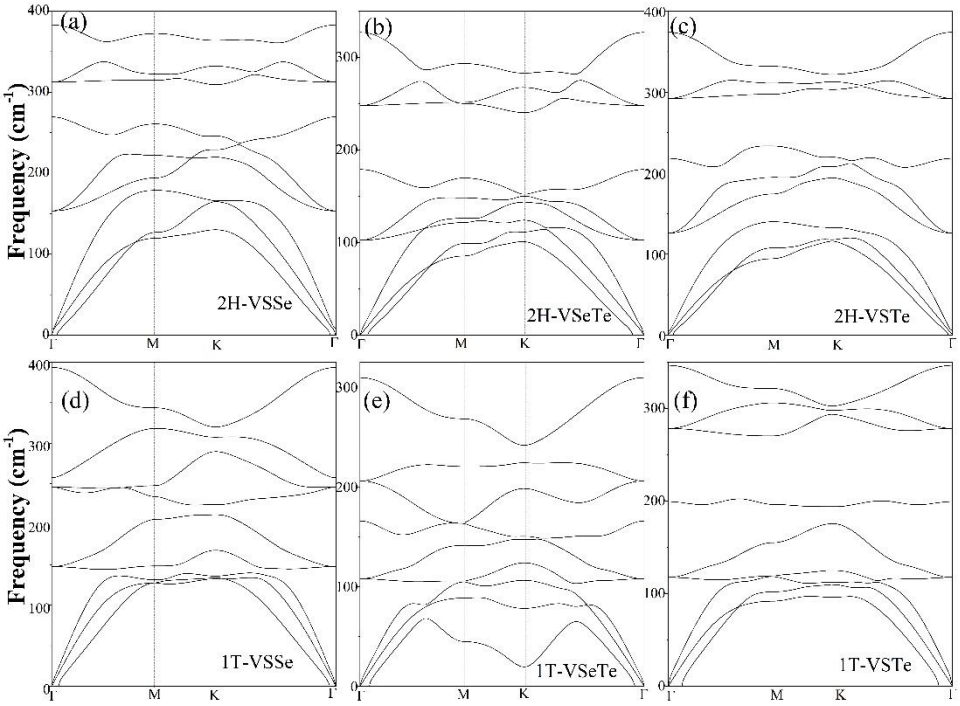

Fig. S2. The phonon spectrum calculations for the six Janus-VXX'. It can be clearly seen that the phonon spectra of the six Janus-VXX' have no imaginary frequency, indicating that they are all dynamically stable and they can exist as free-standing 2D monolayers. Very recently, the Janus MoSSe monolayer has been successfully synthesized. The H_2 is passed into the chamber with MoS_2 to strip and replace the top-layer S atom, and then the Se powder is thermally evaporated to replace the H atom to synthesize the Janus MoSSe monolayer.[1] We believe that the Janus VXX' monolayers can also be prepared in the same way.

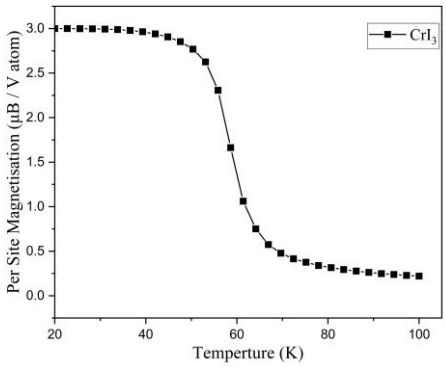

Fig. S3. Per site magnetization of CrI_3 monolayer as a function of temperature. The dark squares are the Monte Carlo simulations. T_c based on our calculation for CrI_3 monolayer is 60 K, which agrees with the experimental result 45 K [2].

Table S2. The exchange coupling constants (*J*) of 1T- and 2H- VXX' monolayers.

	J (meV)		**J (meV)**
1T-VSSe	-5.17	2H-VSSe	-22.62
1T-VSeTe	-20.78	2H-VSeTe	-33.24
1T-VSTe	-16.49	2H-VSTe	-23.34

1T-VS_2	-1.15	2H-VS_2	-17.00
1T-VSe_2	-6.54	2H-VSe_2	-34.79
1T-VTe_2	-13.1	2H-VTe_2	-37.58

Table S3. The magnetic anisotropy energy of 1T- and 2H- VXX' monolayers.

	$E_{in\text{-}plane} - E_{out\text{-}of\text{-}plane}$ (meV / V atom)	
	1T	2H
VSSe	0.052	-0.413
VSeTe	-0.171	-1.094
VSTe	-0.520	-0.768

References

[1] Lu A Y, Zhu H, Xiao J, Chuu C P, Han Y, Chiu M H, Cheng C C, Yang C W, Wei K H, Yang Y, Wang Y, Sokaras D, Nordlund D, Yang P, Muller D A, Chou M Y, Zhang X and Li L J 2017 *Nat Nanotechnol* **12** 744-749.

[2] Huang B, Clark G, Navarro-Moratalla E, Klein D R, Cheng R, Seyler K L, Zhong D, Schmidgall E, McGuire M A, Cobden D H, Yao W, Xiao D, Jarillo-Herrero P and Xu X 2017 *Nature* **546** 270-273.