Supporting Information for

Two-dimensional honeycomb-kagome V_2X_3 (X = O, S, Se) with half-metallicity, high Curie temperature and large magnetic anisotropic energy

Sai Ma,[1,*] Xiangyan Bo, [1,*] Lei Fu,[1] Xiaoyu Liu, [1] Suen Wang,[1] Mengxian Lan,[1] Shasha Li,[1] Tian Huang,[1,†] Feng Li,[1,†] and Yong Pu[1,†]

[1]*School of Science & New Energy Technology Engineering Laboratory of Jiangsu Province, Nanjing University of Posts and Telecommunications (NJUPT), Nanjing 210046, China*

Sai Ma and Xiangyan Bo contributed equally to this manuscript.

Corresponding Authors: lifeng@njupt.edu.cn; puyong@njupt.edu.cn

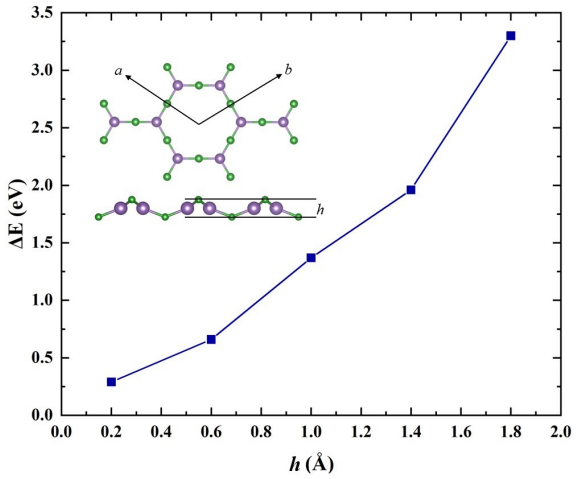
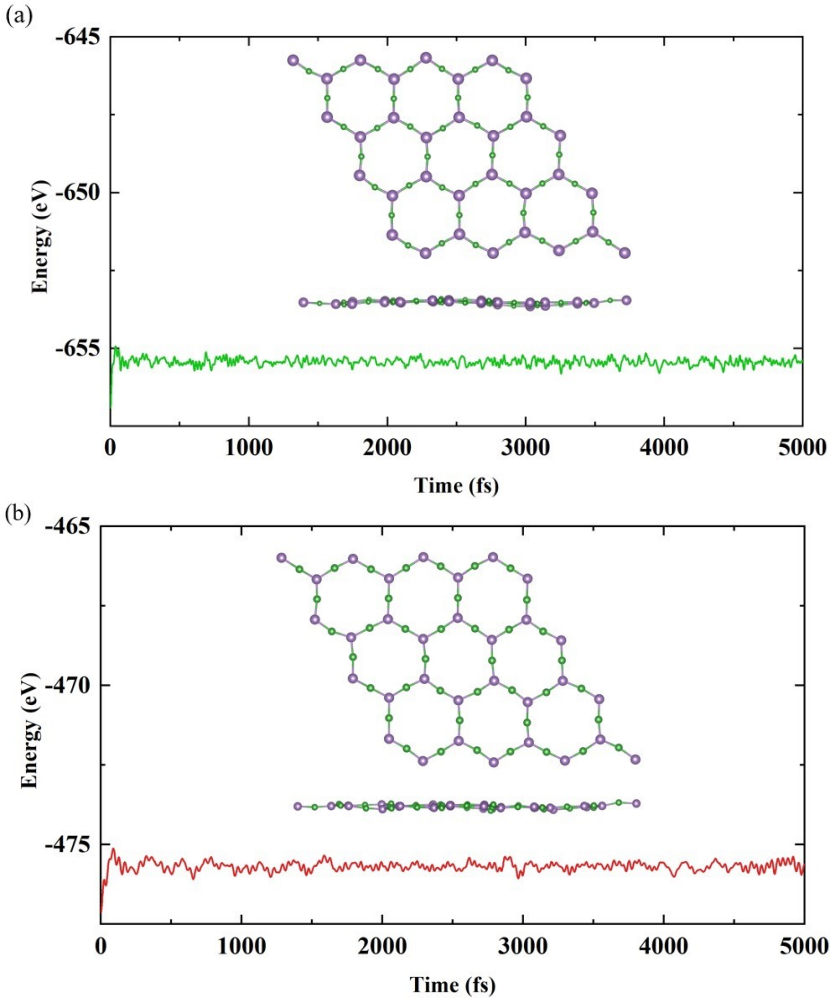


Figure S1: The variation of total energy difference, $\Delta E = E_{(Buckled)} - E_{(Planar)}$, as a function of buckled height h. The insets are buckled V_2O_3 lattice. It can be seen that the planar structure has the lowest energy and, hence, is most stable.



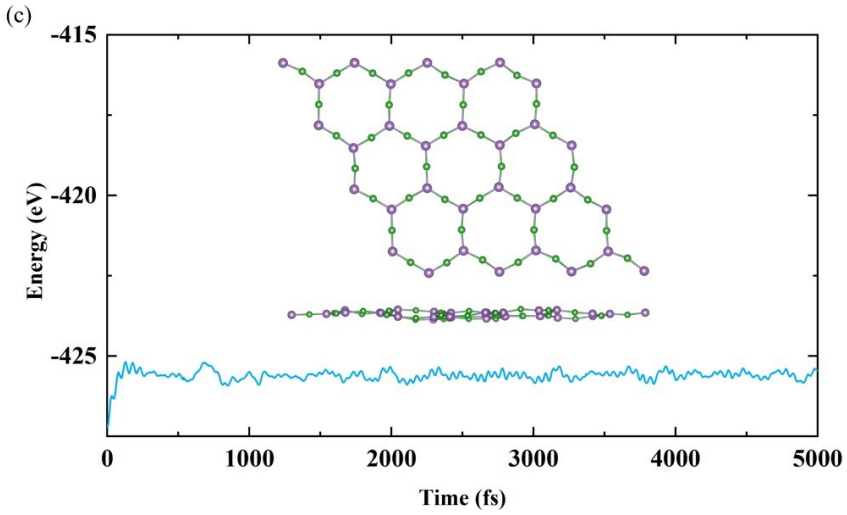
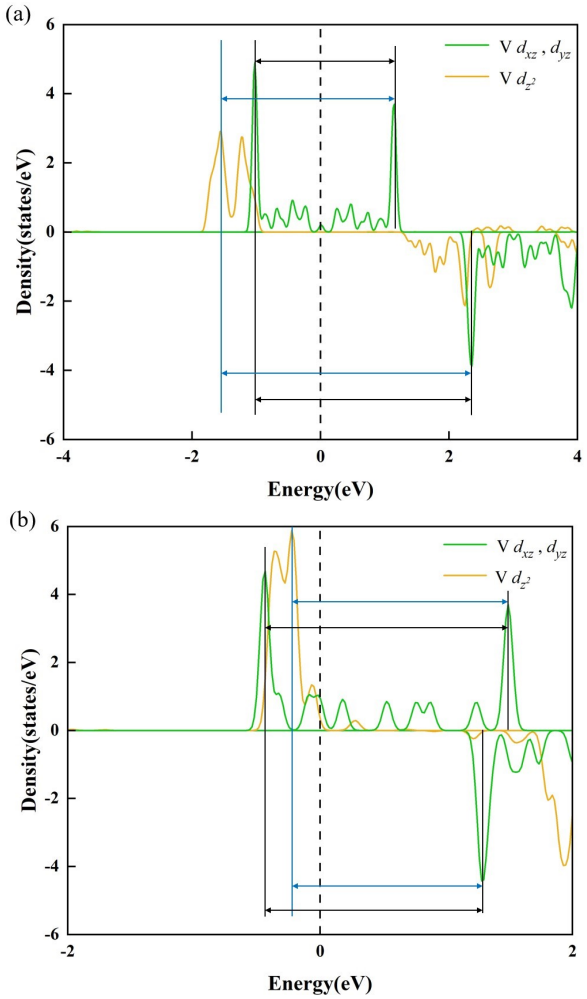


Figure S2: The evolution of total energy of the V_2X_3 (X = O, S, Se) monolayers as a function of time at 300 K.



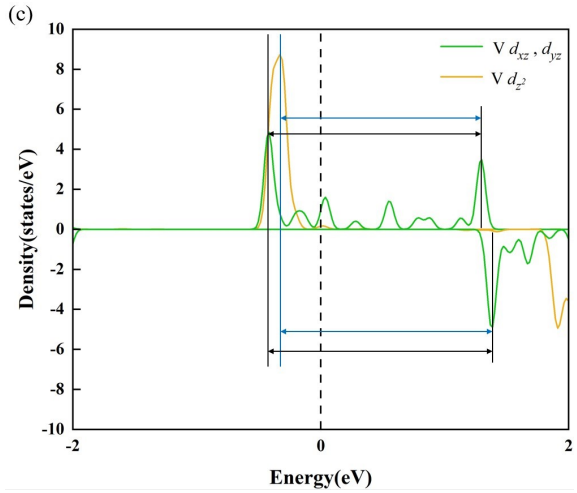


Figure S3: PDOS of V-d_{xz}/d_{yz} and V-d_z^2 orbitals of (a) V_2O_3, (b) V_2S_3, and (c) V_2Se_3.

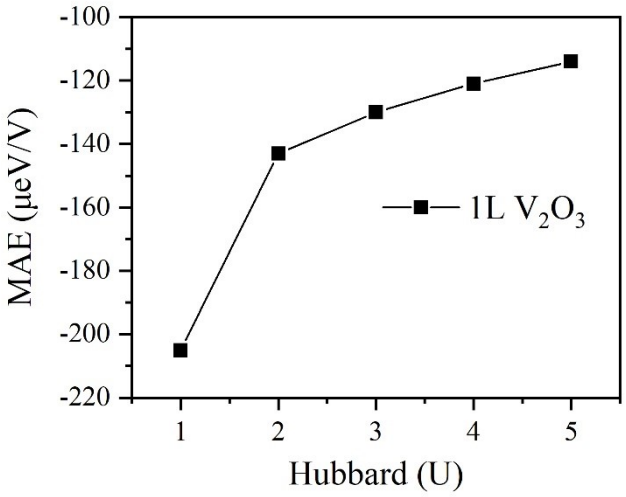


Figure S4. The energy difference between the FM state of monolayer V_2O_3 along the 001 and 100 directions as a function of the Hubbard *U* value.