Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Two-dimensional Ferroelectric Ferromagnetic Half Semiconductor in VOF monolayer

Shaowen Xu[a], Fanhao Jia[a], Guodong Zhao[a] Wei Wu[a], and Wei Ren[a†]

[1]*Physics Department, Shanghai Key Laboratory of High Temperature Superconductors, State Key Laboratory of Advanced Special Steel, International Centre of Quantum and Molecular Structures, Shanghai University, Shanghai 200444, China*

[†]renwei@shu.edu.cn

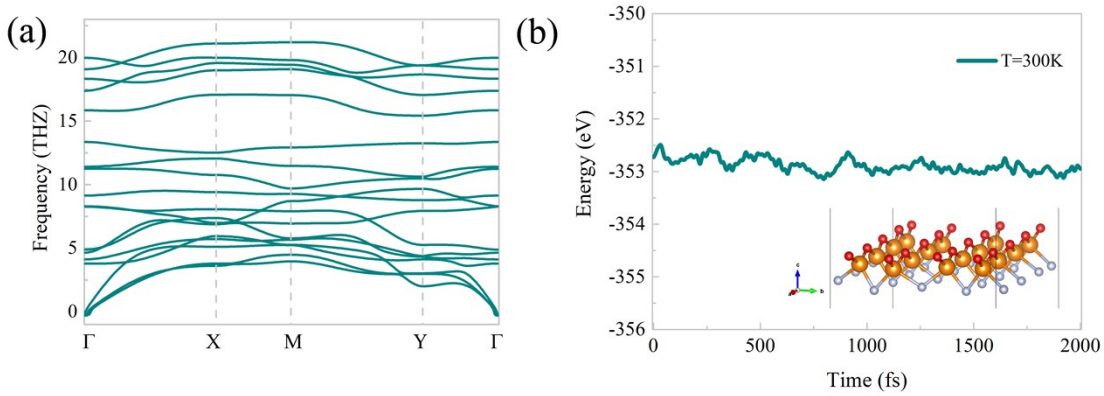

Figure S1 (a) The phonon spectra of the VOF monolayer. (b) The evolution of energy over time at T=300 K from molecular dynamics simulations of VOF monolayer.

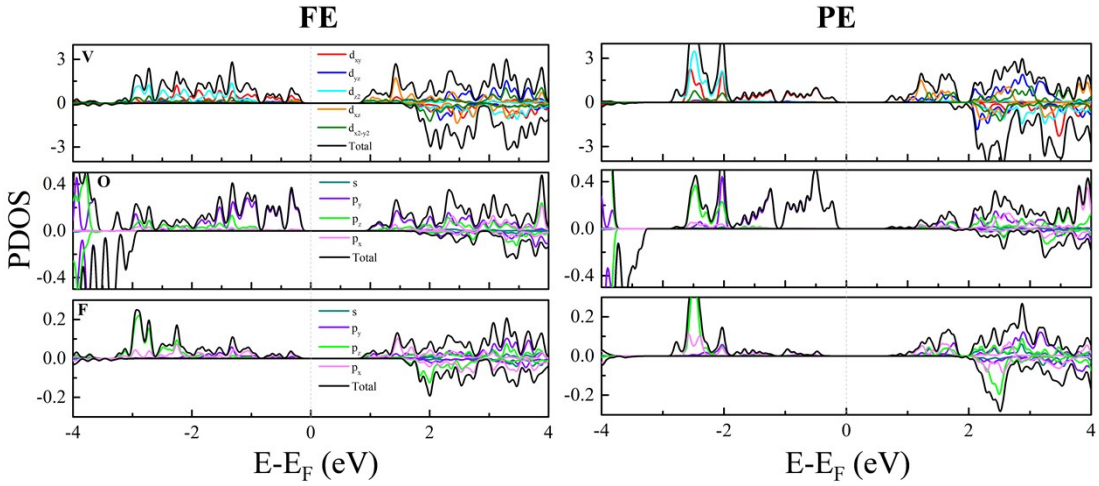

Figure S2. The HSE06 partial density of states (PDOS) of ferromagnetic VOF monolayer of FE and PE states. The Fermi energy level is set to zero.

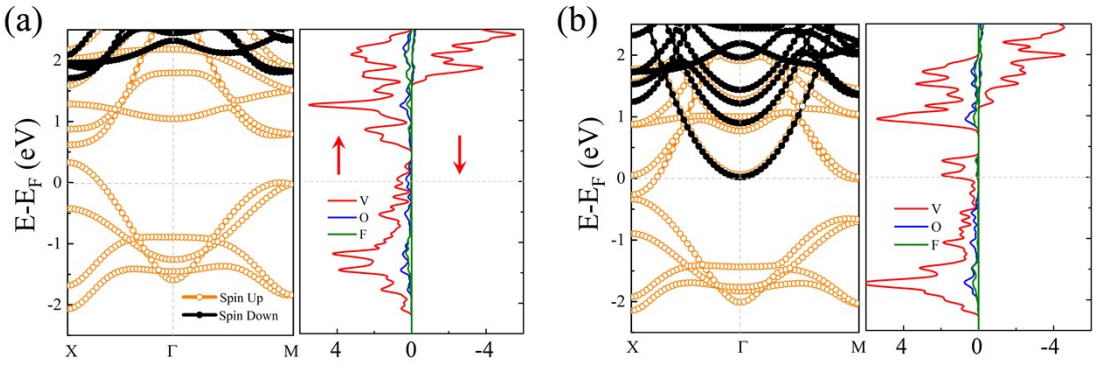

Figure S3 The electronic structures of VOF monolayer with (a) hole and (b) electron doping density of 0.1/formula unit.

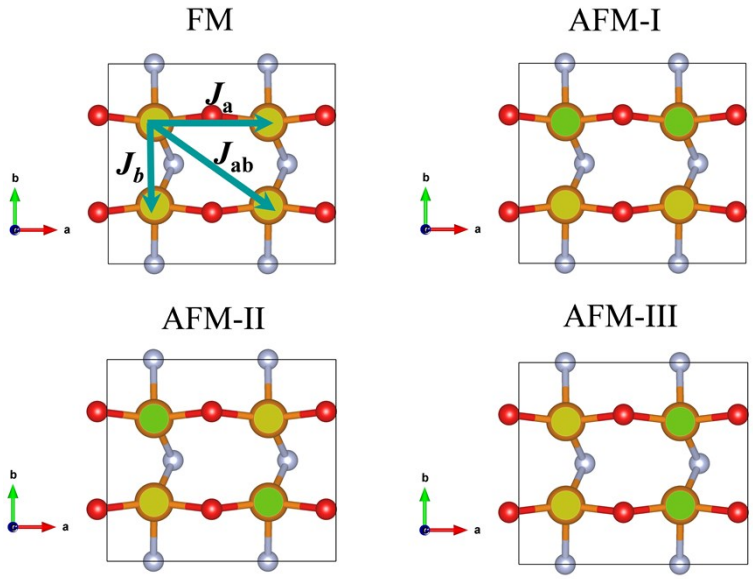

Figure S4 Spin density distributions for the VOF monolayer under different magnetic configurations, the yellow and green balls represent the spin up and spin down states.

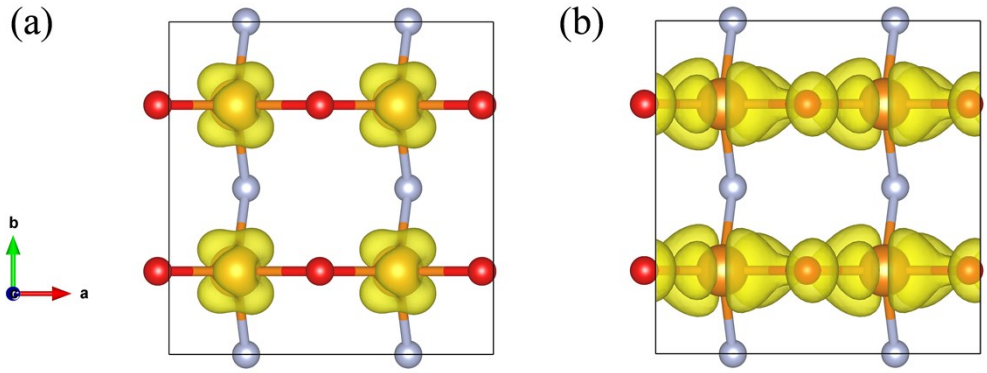

Figure S5 (a)The spin density and (b) wavefunction of the valence band maximum at the gamma point of VOF monolayer.

Table SI The elastic constants (N/m) of VOF monolayer.

C_{11}	C_{12}	C_{22}	C_{66}
90.876	-8.686	26.117	1.124

Table SII: The energy gap (eV), local magnetic moment per V atoms (μ_B) and the energy difference ΔE (meV) between FM and AFM (E_{FM}-E_{AFM}) of VOF monolayer calculated by HSE06 method.

Configuration	Gap	Type	M	ΔE
FM	1.672	direct	1.930	0
AFM-I	2.143	direct	1.912	-25.2
AFM-II	2.959	direct	1.814	-180
AFM3-III	2.858	direct	1.828	-153