Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Multiferroic vanadium phosphide monolayer with ferromagnetic half-metallicity and topological Dirac states

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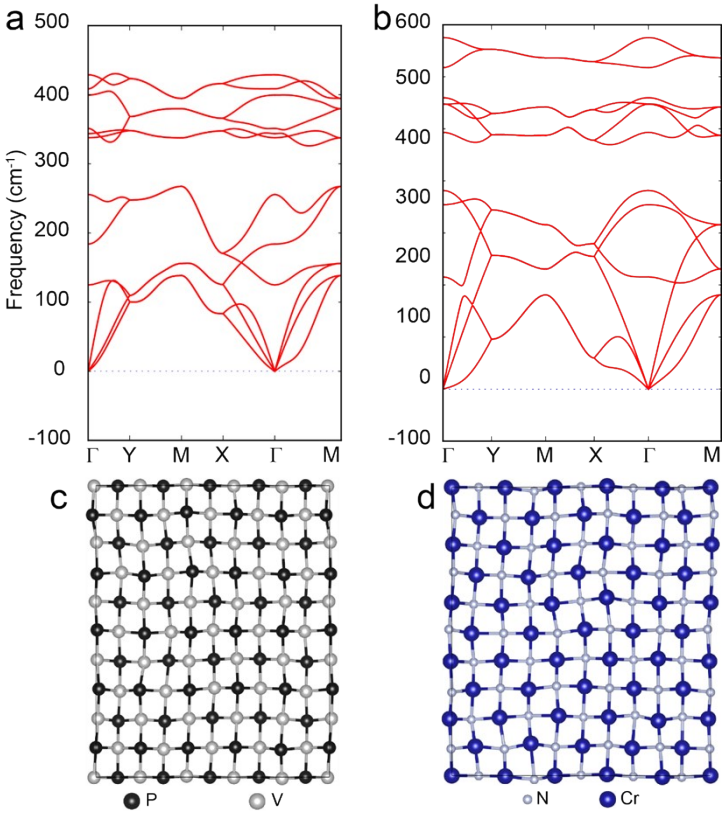

Figure S1. (a, b) Calculated phonon spectra of the t-VP and t-CrN monolayers. (c, d) Snapshots of the two monolayers at the end of 10 ps ab initio molecular dynamics simulations at 500 K.

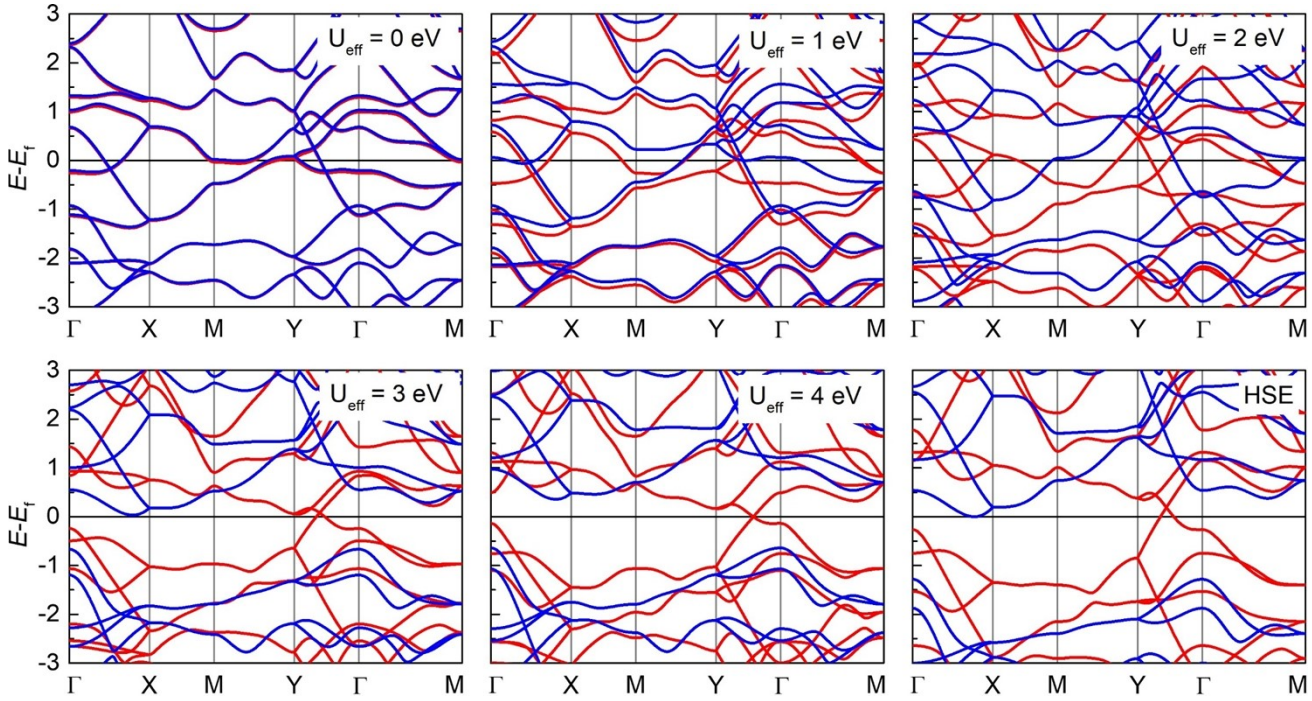

Figure S2. Band structures of the t-VP monolayer without the SOC calculated with the DFT+U method (the values of U_{eff} are provided) and HSE06 functional. The red and blue lines present the spin-up and spin-down band structures, respectively.

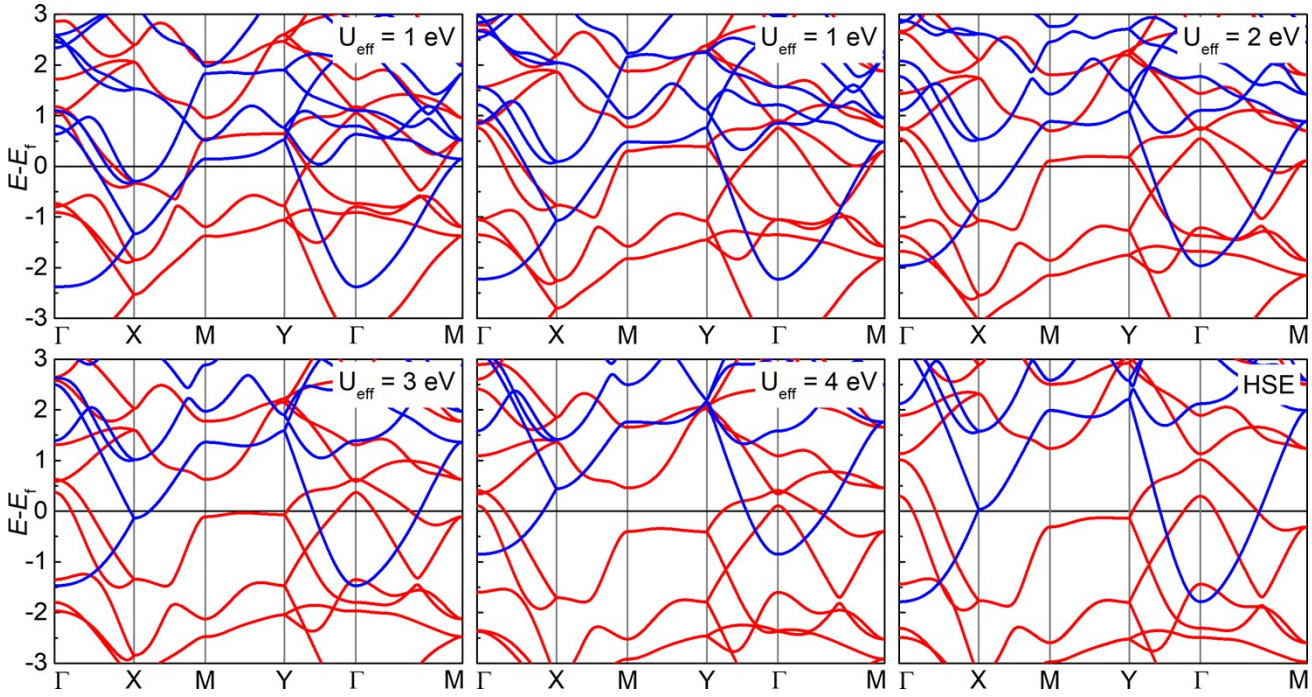

Figure S3. Band structures of the t-CrN monolayer without the SOC calculated with the DFT+U method (the values of U_{eff} are provided) and HSE06 functional. The red and blue lines present the spin-up and spin-down band structures, respectively.

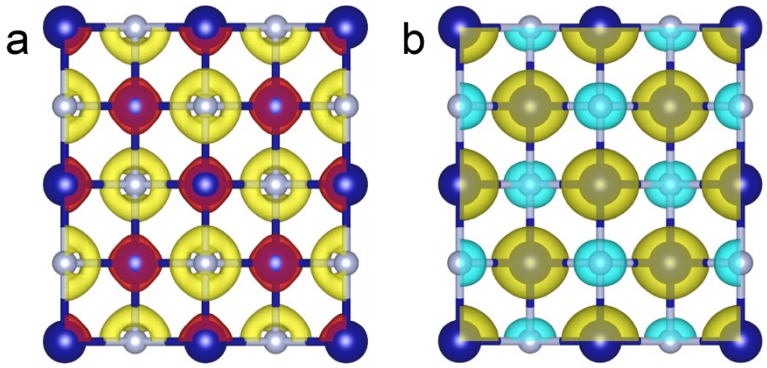

Figure S4. Isosurface plots of deformation electronic density (a, 0.134 e/Å^3) and spin polarization distribution (b, 0.134 e/Å^3) of the t-CrN monolayer. Bader charge analysis shows that a charge transfer of 0.60 e from each Cr atom to N atom (from deep red to yellow). The transferred electrons in the t-CrN monolayer are mainly from 3 $d_{xz,yz}$ orbitals of Cr atoms and delocalize around N atoms in 3 $p_{x,y}$ orbitals.

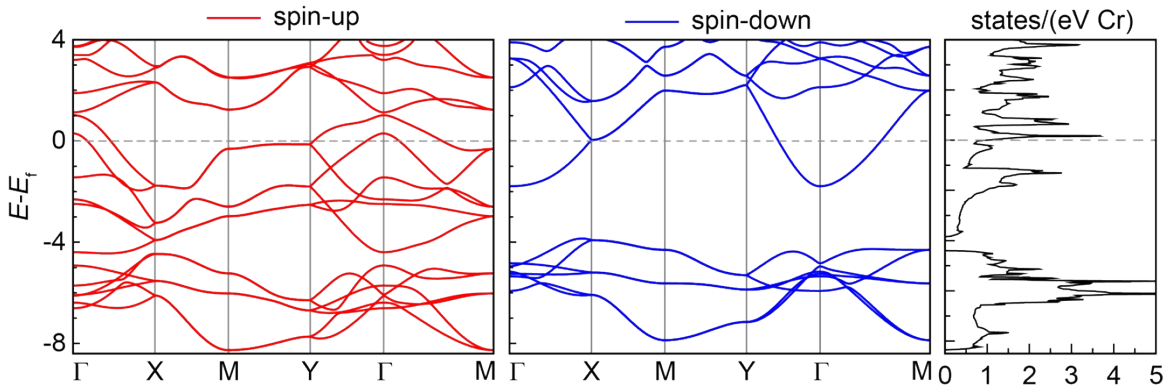

Figure S5. Spin-polarized band structures and density of states of the t-CrN monolayer in its non-magnetic state, calculated with the HSE06 functional.