Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Proton-transfer Ferroelectricity / Multiferroicity in Rutile Oxyhydroxides

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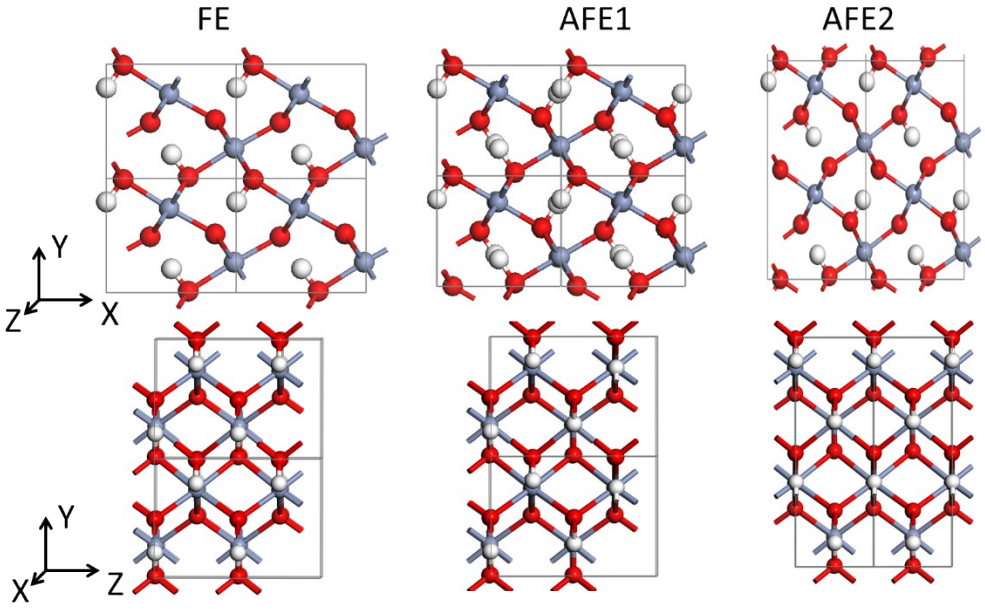

Figure S1 Geometric structures of FE (left) and two configurations that are antiferroelectric respectively along the -Z axis and -Y axis (AFE1 middle, and AFE2 right) for CrOOH, where the antiferroelectric states are respectively 0.067eV and 0.09eV higher compared with FE state.

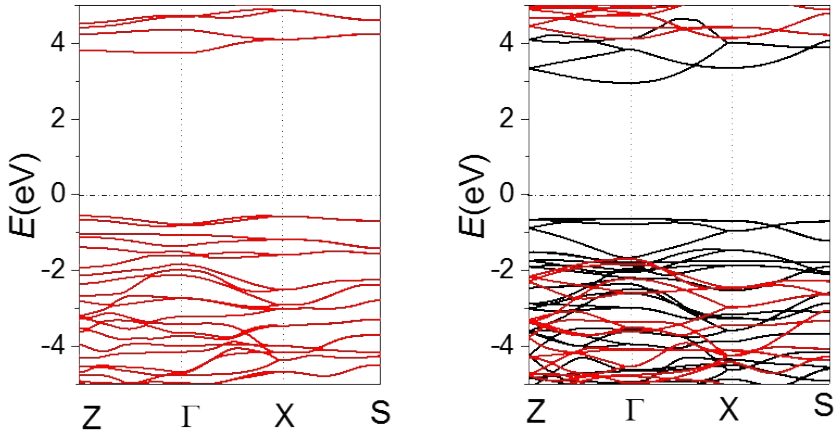

Figure S2 Bandstructures of CrOOH upon zero (left) and 2% strain in z direction (right), which is calculated by using HSE06 functional.

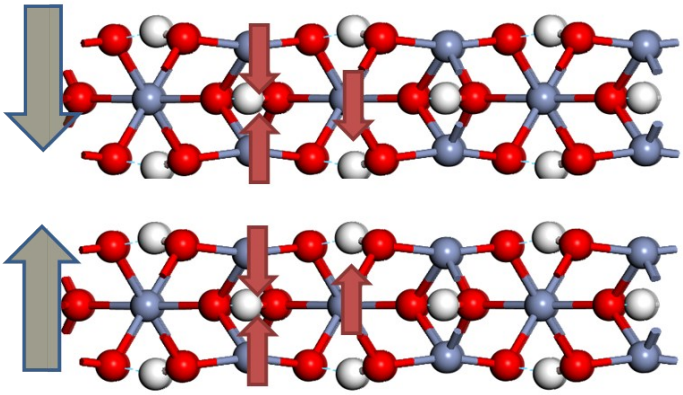

Figure S3 Vertical ferroelectric switching upon ferrimagnetic switching in a thin layer of CrOOH isolated from (001) surface. Different spin configurations are compared and the displayed ferrimagnetic state turns out to be the ground state.

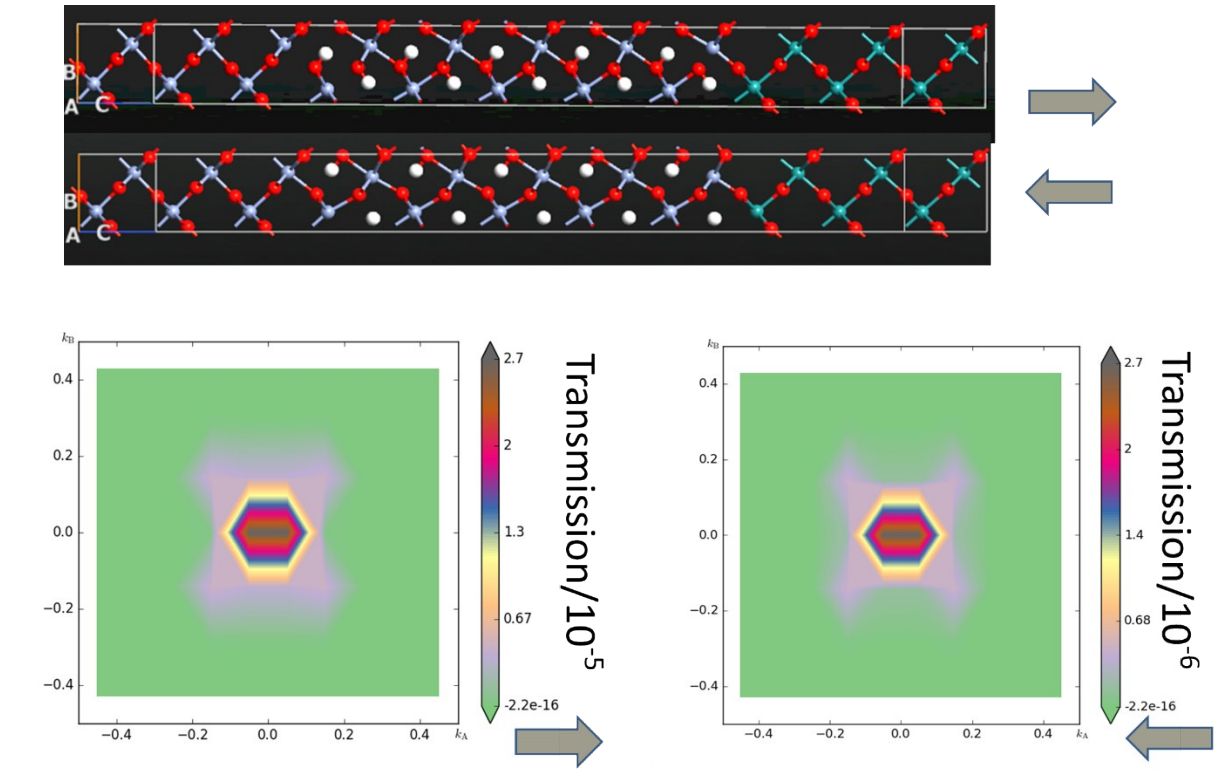

Figure S4 Model of MTJ composed of CrO_2/CrOOH/RuO_2 and k-resolved transmission spectrums.

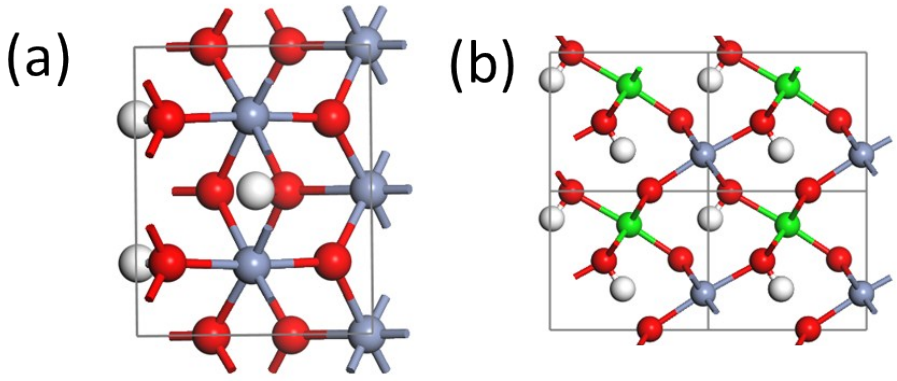

Figure S5 Geometric structures of (a) $CrOOH_{0.75}$ and (b) $Cr_{0.5}Fe_{0.5}OOH$.

Table S1. Energy difference $\Delta E = E(\text{FM}) - E(\text{AFM2})$ for $CrOOH_x$.

x in $CrOOH_x$	0.25	0.5	0.75	1
ΔE(meV/f.u.)	-106.0	-75.1	-33.0	30.1