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Supporting Information for

Remarkable ferroelectricity—modulated electronic and magnetic properties in a 2*H*–VS₂/BiAlO₃(0001) hybrid system

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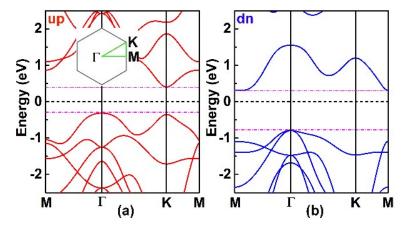


Fig. S1 Band structures in primitive–cell Brillouin zone of the pristine 2*H*–VS₂. Here, (a) and (b) demonstrate the spin–up and spin–down channel, respectively, the energy scale is labeled with respect to the Fermi level, and the inset of Fig. S1a shows the First Brillouin zone of the hexagonal primitive–cell of the 2*H*–VS₂.

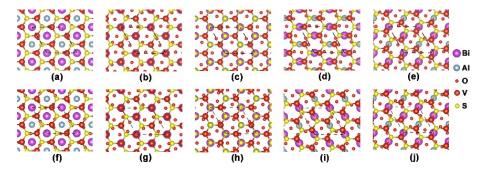


Fig. S2 Five typical interface configurations of the (a–e) 2H-VS₂/BAO Z+ and (e–h) 2H-VS₂/BAO Z- systems (top views). For clarity, Only the surface termination, outer one -Al-O₃-Bi- trilayer (-Al-Bi-O₃- trilayers for BAO Z- surface), and the 2H-VS₂ overlayer are plotted.

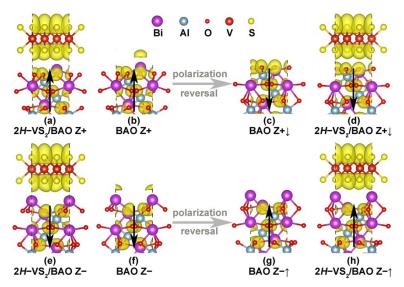


Fig. S3 ELFs (side views) of the (a) 2H– VS_2/BAO Z+, (d) Z+ \downarrow , (e) Z-, and (h) Z- \uparrow systems as well as the clean (b) BAO Z+, (c) Z+ \downarrow , (f) Z-, and (g) Z- \uparrow surfaces (the plotted isosurface is 0.5 e/ų). Here, the black arrow denotes the ferroelectric polarization direction.