Supporting Information

Enhanced stability and stacked dependent magnetic/electronic properties of 2D monolayer $FeTiO_3$ on Ti_2CO_2 substrate

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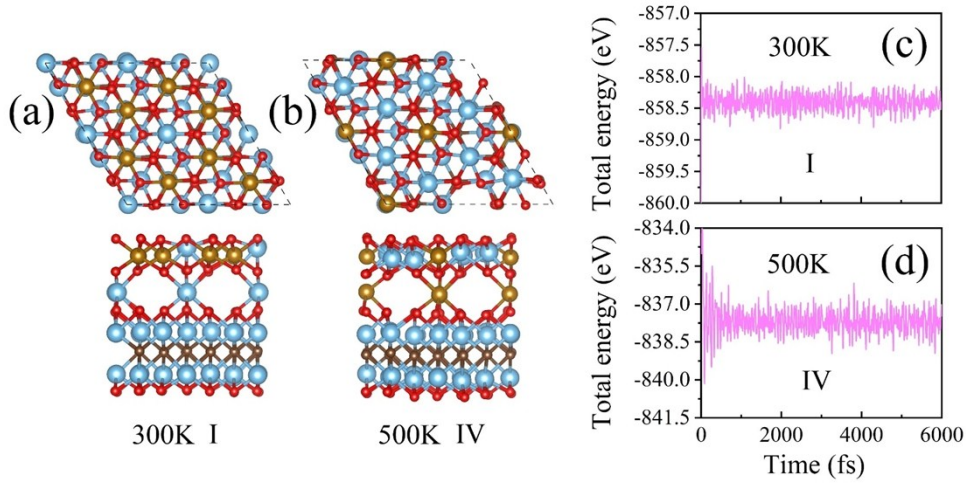

Fig. S1 Left panel: structural snapshots for 2 × 2 $FeTiO_3/Ti_2CO_2$ (100 atoms) configuration I (a) at 300 K, and configuration IV (b) at 500 K within 6 *p*s during AIMD simulation; Right panel: variation of the total energy for configuration I (c) and configuration IV (d) at time of 6 *p*s along AIMD simulation under the temperatures of 300 K and 500K, respectively.

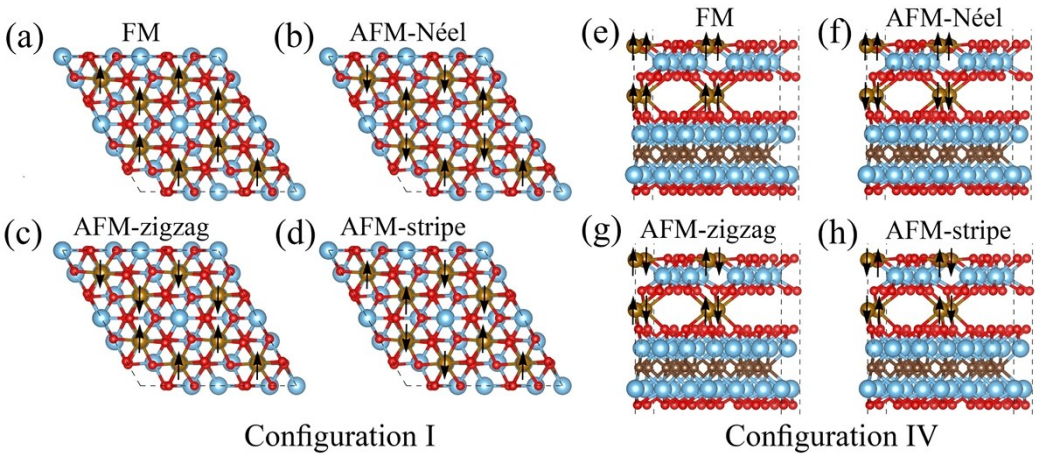

Fig. S2 Left panel: top view of the FM (a), and various AFM spin configurations: AFM-Néel (b), AFM-zigzag (c), AFM-stripy (d) of configuration I with 2 × 2 supercell. Right panel: the side view of the FM (a), AFM-Néel (b), AFM-zigzag (c), and AFM-stripy (d) of configuration IV with 2 × 2 supercell. Blue, gray, red and brown balls are Ti, C, O and Fe atoms, respectively. Up and down arrows denote the spin-up and down polarization of Fe atoms, respectively.

Tab. S1 The relative energies per unit cell (E_{ex}, in eV) between ferromagnetic (FM), three antiferromagnetic (AFM-Néel, AFM-zigzag, and AFM-stripe) states for 2D $FeTiO_3/Ti_2CO_2$ heterostructure with 2 × 2 supercell. Ground states are highlighted with yellow.

Configuration	FM	AFM-Néel	AFM-zigzag	AFM-stripe
I	0	-0.15	-0.09	-0.13
II	0	0.24	0.01	0.02
III	0	-0.07	-0.03	-0.05
IV	0	0.01	0.10	0.04
V	0	-0.01	-0.02	0.07
VI	0	-0.02	-0.01	-0.03

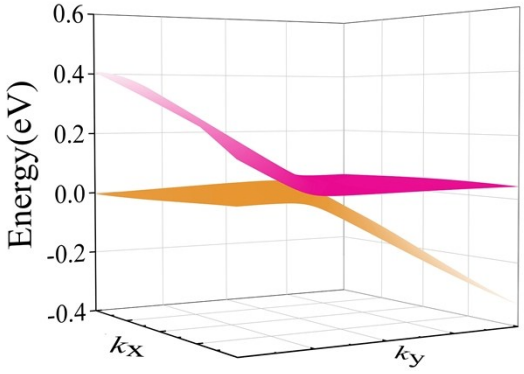

Fig. S3 The 3D band structure around the Fermi level of 2D $FeTiO_3/Ti_2CO_2$ configuration IV along the M-G direction in the Brillouin zone.

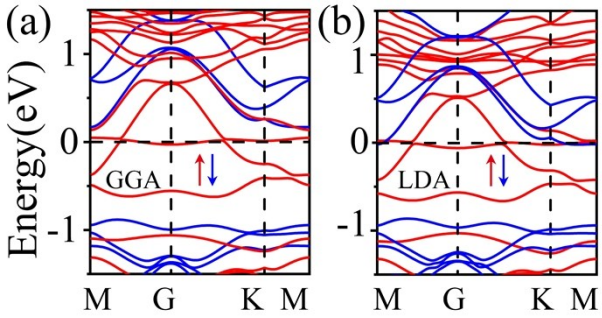

Fig. S4 Spin-polarized band structures of 2D $FeTiO_3/Ti_2CO_2$ configuration IV with the (a) GGA+U method, and (b) LDA+U method. Red and blue lines (arrows) denote spin-up and spin-down bands, respectively. Dashed lines refer to the Fermi level set to zero.