Identification of Atomic Defects and Adsorbate on Rutile TiO$_2$(110)-(1×1) Surface by Atomic Force Microscopy

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Figure S1. Ball model of rutile TiO$_2$ (110)-(1×1) surface with top view (a) and side view (b).
Figure S2. AFM images (a-d) of TiO$_2$(110)-(1×1) surface with different image contrast mode by Si tip termination. (a) Recorded in the hole mode. (b) Recorded in the protrusion mode. (c) Tip jumped during upward scanning. Down and upper parts are recorded in the hole and protrusion mode, respectively. (d) Imaging contrast can be changed back and forth during the imaging process.
Figure S3. AFM images of TiO$_2$(110)-(1×1) surface in the same area at various tip-sample distance. (Note: the row direction for four images is different due to the upward and downward scanning direction) (a)-(b) can be attributed to the hole and protrusion mode, respectively. (c) Recorded in the neutral mode. (d) is obtained in the variable tip-sample distance during the imaging process. ($f_0 = 802$ kHz, $Q = 19738$, $V_{DC} = 0.6$ V, $A = 500$ pm, $10 \times 10$nm$^2$)
Figure S4. (a) and (c) AFM images of TiO$_2$(110)-(1×1) surface in the same area with different tip structure. (b) and (d) line profiles cross O$_V$ and OH along the [001] direction, taken in (a) and (c), respectively. ($f_0 = 803$ kHz, $Q = 32240$, $V_{DC} = 1$ V, $A = 500$ pm, $3 \times 4$ nm$^2$).
Figure S5. (a)-(c) AFM images of O-TiO$_2$(110)-(1×1) surface in the same area. (d) and (e) KPFS performance taken at the same point in (a). (f) KPFS performance taken in (b). ($f_0 = 803$ kHz, $Q = 32240$, $V_{DC} = 1$ V, $A = 500$ pm, $7 \times 7$ nm$^2$).