

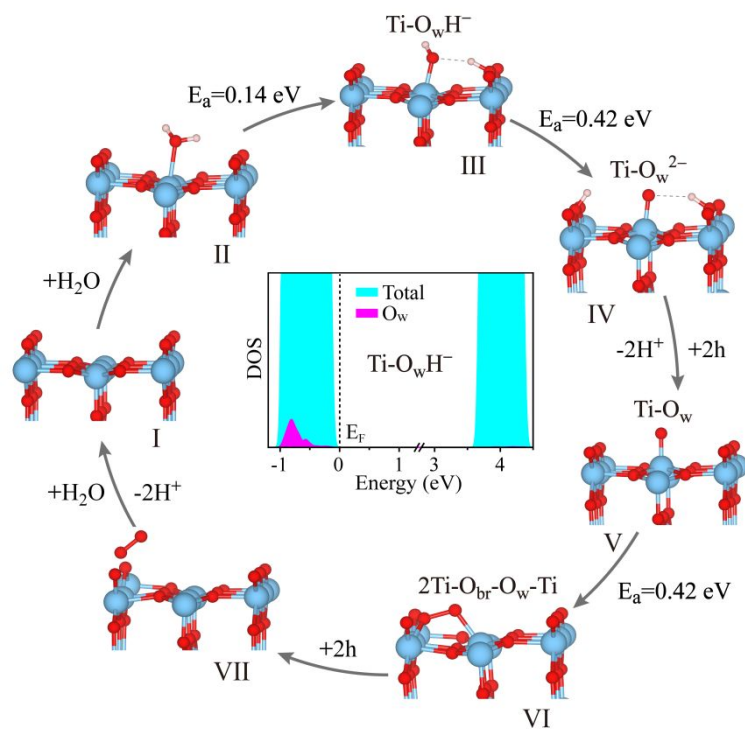
**Supporting Information for**

**Reaction Pathway of Photocatalytic Water  
Splitting on Two-Dimensional TiO<sub>2</sub> Nanosheets**

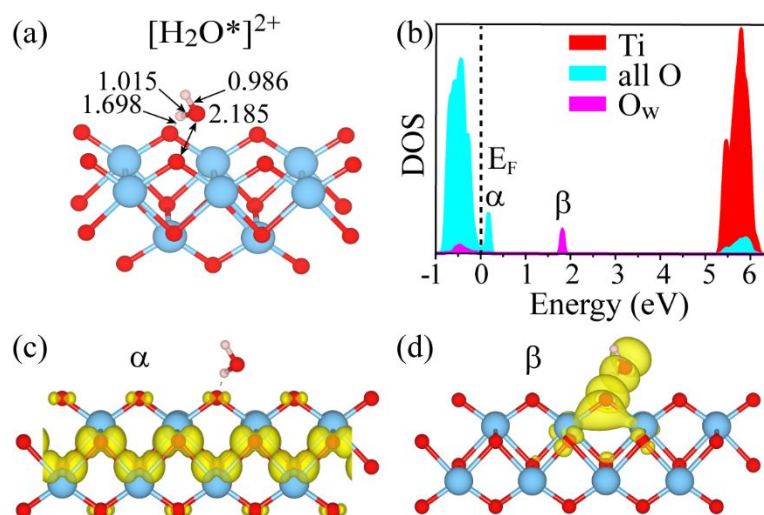
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School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, China

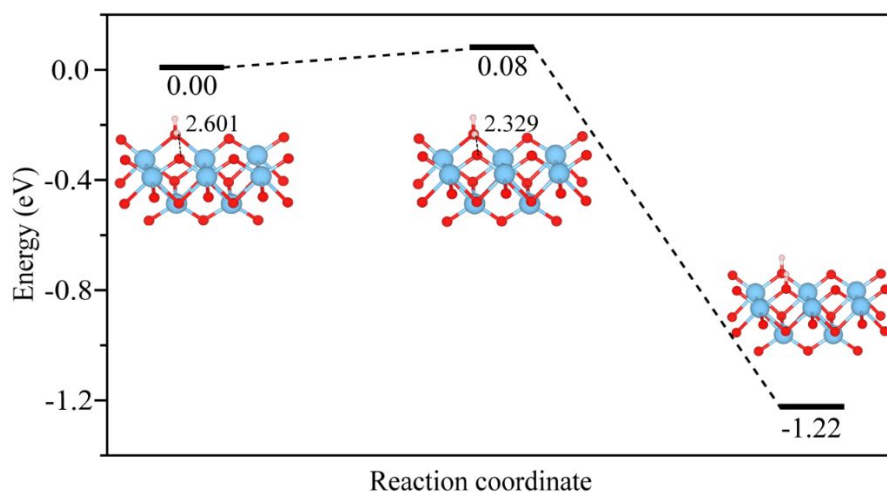
Corresponding Author: myc@sdu.edu.cn



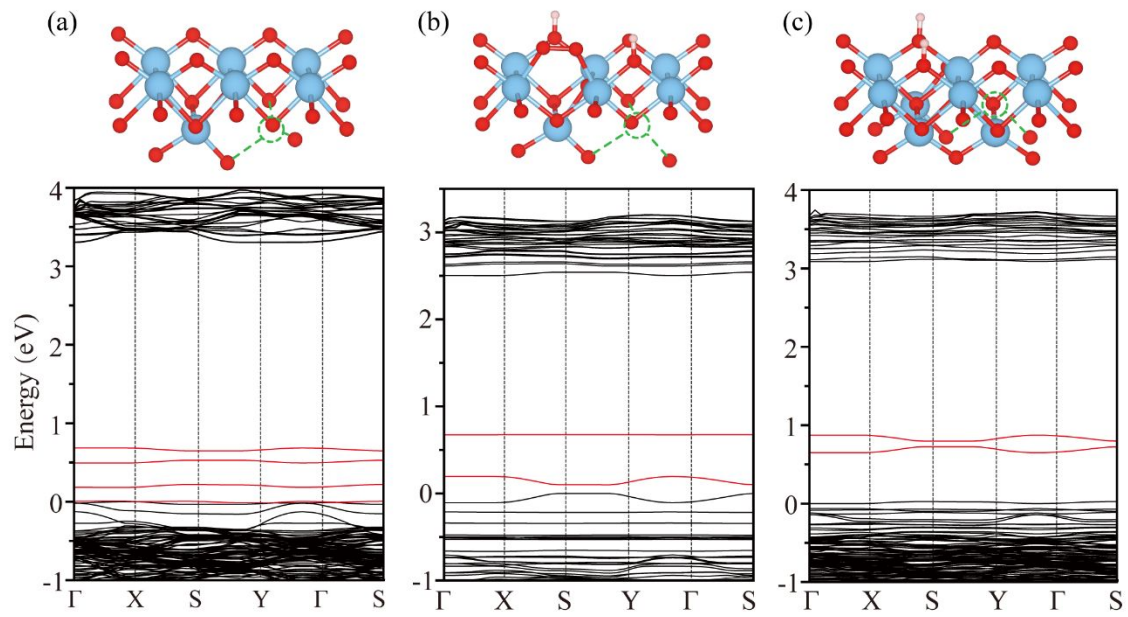
**Figure S1.** Reaction mechanism for photocatalytic water splitting on the rutile  $\text{TiO}_2(110)$  surface as reported in our previous work published in J. Mater. Chem. A 9, 7650 (2021). The total and projected electronic DOSs calculated by GW for the configuration  $\text{Ti-O}_w\text{H}^-$  are shown in the central panel in which the reference energy is set to VBM and the black dashed line marks the Fermi level.



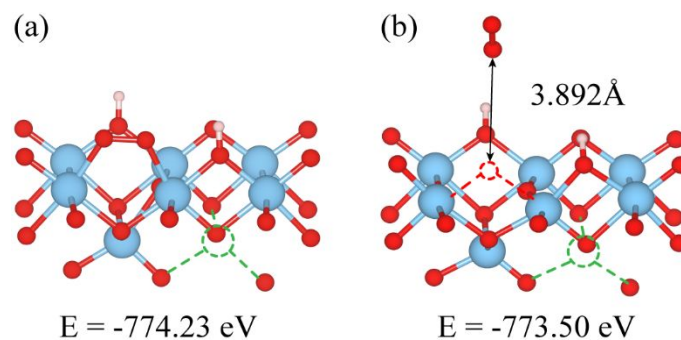
**Figure S2.** The geometry (a) and the projected electronic DOS calculated by GW (b) for  $[\text{H}_2\text{O}^*]^{2+}$ . (c) [(d)] Hole distribution at the density of  $0.01 \text{ e}/\text{\AA}^3$  for the peak  $\alpha$  [ $\beta$ ] marked in (b). The reference energy and the black dashed line in DOS marks VBM and the Fermi level respectively.



**Figure S3.** Potential energy diagram (in eV) for the dissociation of H<sub>2</sub>O at O<sub>v</sub><sup>2+</sup> on the defect-free L-TiO<sub>2</sub>. The black dashed line links one H in H<sub>2</sub>O and one O<sub>br</sub>, and the corresponding interatomic distance (in Å) is shown as well.



**Figure S4.** Geometries (top panels) and band structures calculated by DFT+ $U$  (bottom panels) for the L-TiO<sub>2</sub> containing a Ti<sub>v</sub>. (a) Clean surface. (b) Ti-O<sub>w</sub>O<sub>br</sub>-Ti+2H. (c) Ti<sub>v</sub>+2H. The green dashed circles and dashed lines indicate positions of the Ti vacancy and the original Ti-O bonds, respectively. VBM is set to zero. The empty levels within the band gap are highlighted in red.



**Figure S5.** (a) Geometry and total energy of Ti-O<sub>w</sub>O<sub>br</sub>-Ti+2H on the L-TiO<sub>2</sub> containing a Ti<sub>v</sub>. (b) Geometry and total energy after the O<sub>w</sub>-O<sub>br</sub> group in Ti-O<sub>w</sub>O<sub>br</sub>-Ti+2H of (a) escapes L-TiO<sub>2</sub>, forming a O<sub>2</sub> molecule and leaving a O<sub>v</sub> behind. The green (red) dashed circles and dashed lines indicate positions of the Ti (O) vacancy and the original Ti-O bonds, respectively.

# Atomic coordinates for the configurations discussed in the context

| States | Configurations                                             |
|--------|------------------------------------------------------------|
| 1      | Defect-free                                                |
| 2      | $\text{H}_2\text{O}^*$                                     |
| 3      | $[\text{H}_2\text{O}^*]^+$                                 |
| 4      | $[\text{H}_2\text{O}^*]^{2+}$                              |
| 5      | $\text{Ti-O}_w\text{H-Ti+H}$                               |
| 6      | $[\text{Ti-O}_w\text{H-Ti+H}]^+$                           |
| 7      | $[\text{Ti-O}_w\text{H-Ti+H}]^{2+}$                        |
| 8      | $\text{Ti-O}_w\text{O}_{br}\text{-Ti+2H}$                  |
| 9      | $[\text{Ti-O}_w\text{O}_{br}\text{-Ti+2H}]^+$              |
| 10     | $[\text{Ti-O}_w\text{O}_{br}\text{-Ti+2H}]^{2+}$           |
| 11     | $\text{Ti-O}_w\text{O}_{br}\text{-Ti}$                     |
| 12     | $[\text{Ti-O}_w\text{O}_{br}\text{-Ti}]^+$                 |
| 13     | $[\text{Ti-O}_w\text{O}_{br}\text{-Ti}]^{2+}$              |
| 14     | $\text{O}_v^{2+}$                                          |
| 15     | $\text{O}_v^{2+}+\text{H}_2\text{O}$                       |
| 16     | $\text{O}_v^{2+}+\text{O}_w\text{H}+\text{O}_{br}\text{H}$ |
| 17     | $\text{Ti}_v$                                              |
| 18     | $\text{H}_2\text{O}^*$                                     |
| 19     | $\text{Ti-O}_w\text{O}_{br}\text{H-Ti}$                    |
| 20     | $\text{Ti-O}_w\text{O}_{br}\text{-Ti+2H}$                  |
| 21     | $\text{O}_v^{2-}$                                          |
| 22     | $\text{O}_v$                                               |
| 23     | $\text{Ti}_v+2\text{H}$                                    |
| 24     | $\text{O}_2+2\text{H}$ in Fig. S5b                         |

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