Supporting Information for

Enhancement of Hole Capture and Water Dissociation on Rutile TiO_2(110) by Intermolecular Hydrogen Bonding: Time-Domain Ab Initio Study

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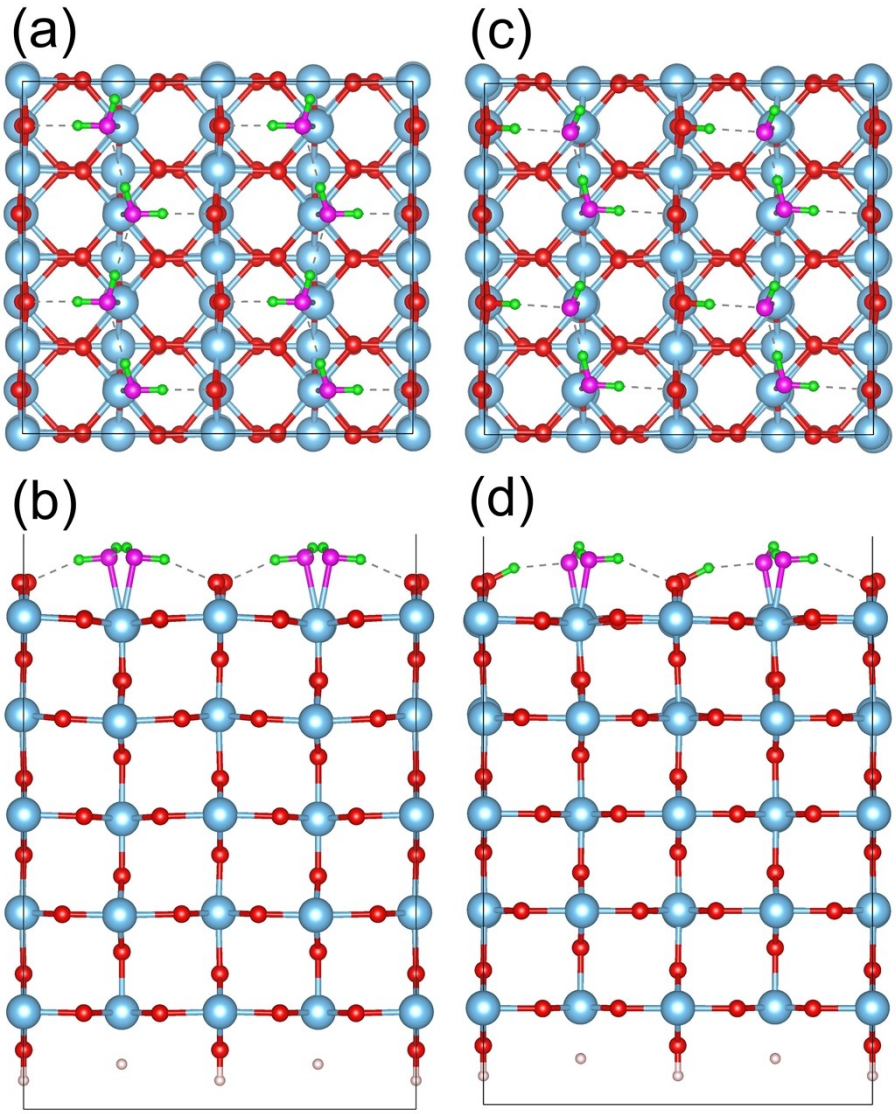

Fig. S1 Adsorption of water molecules on the *p*-rutile TiO_2(110) surface in the 2×2 supercell. **(a, c)** Top and **(b, d)** side views of **(a, b)** monolayer system and **(c, d)** semi-dissociated systems. The light blue and red balls represent Ti and O atoms in TiO_2, respectively, while the pink and green balls represent the O and H atoms in water molecules, respectively.

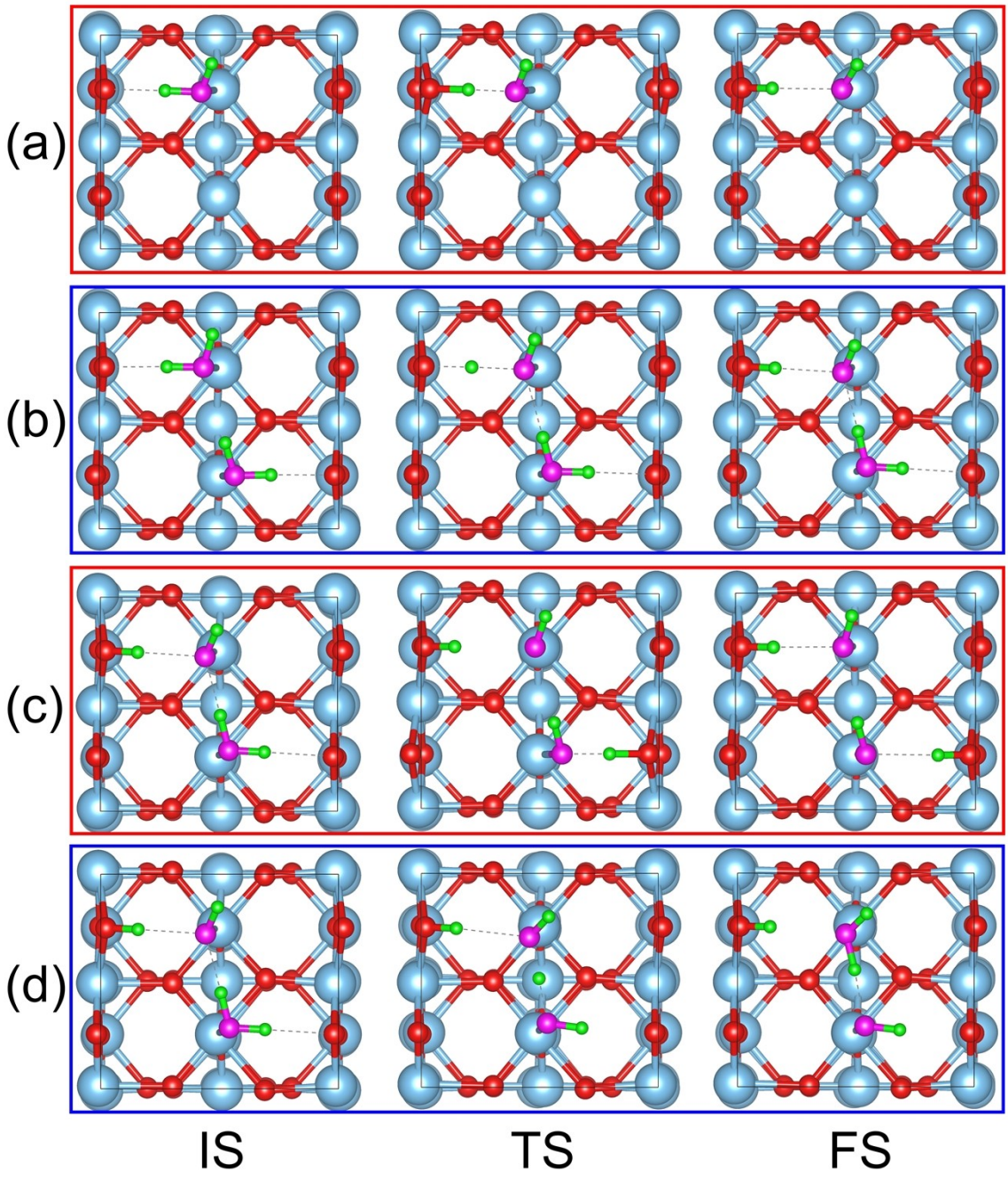

Fig. S2 Enlarged views of the initial state (IS), transition state (TS), and final state (FS) structures corresponding to **Fig. 2**.

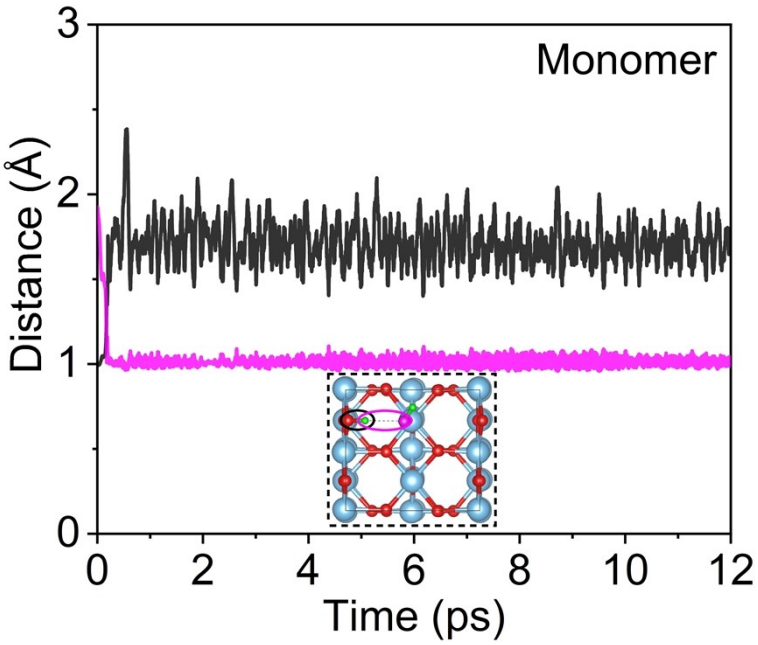

Fig. S3 Evolution of the distances between the H atom and the adjacent O atoms during AIMD in the Monomer system. The evolution of the atomic distances reflects re-formation of the water molecule.

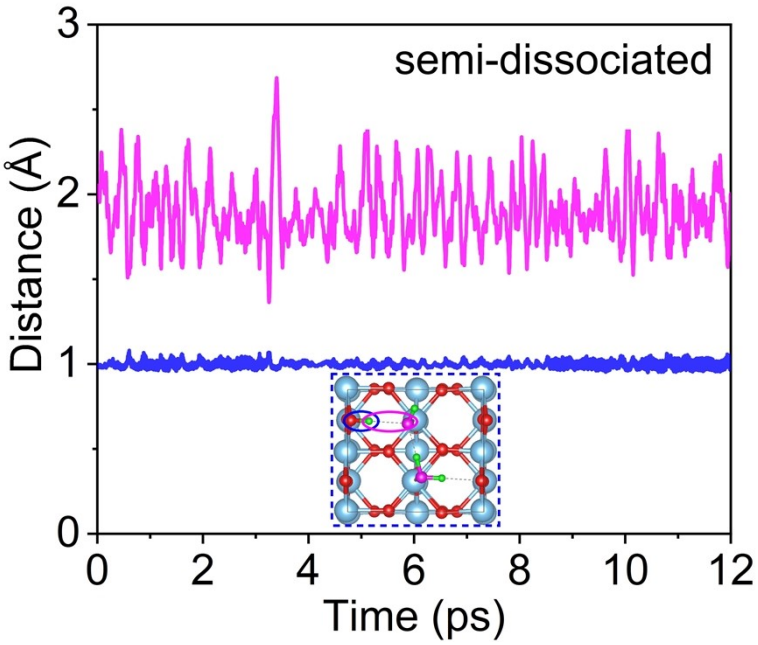

Fig. S4 Evolution of the distances between the H atom and the adjacent O atoms during AIMD in the semi-dissociated system.

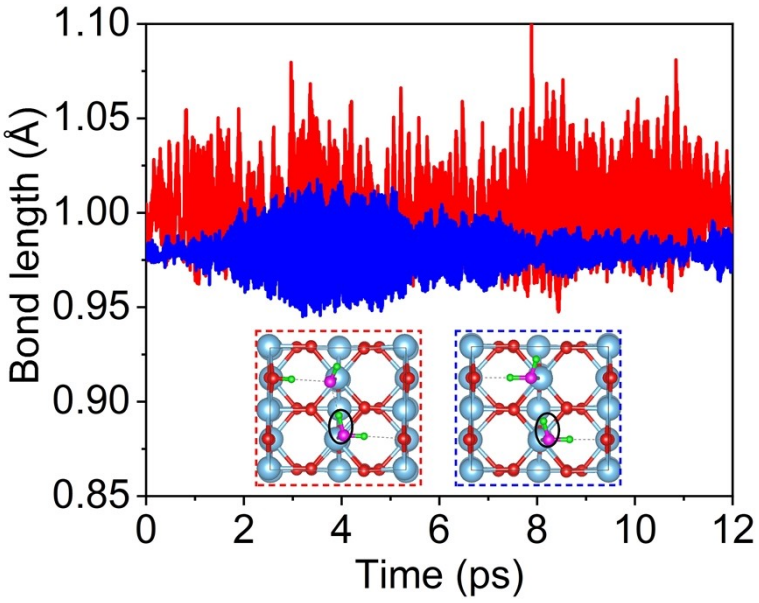

Fig. S5 Evolution of the O-H bond length in the second water molecule H_2O_2 during AIMD in the monolayer (blue) and semi-dissociated (red) systems.