Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Tuning water-splitting mechanism on titanium dioxide surfaces through hydroxylation

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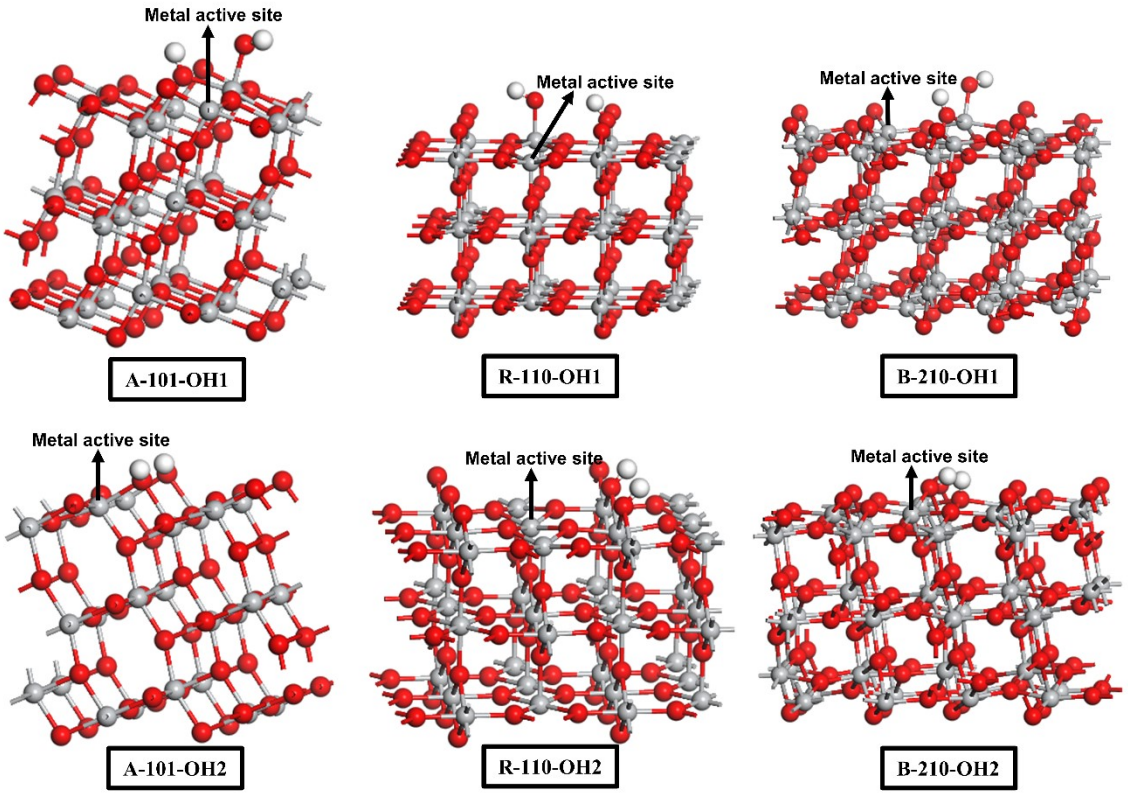

Fig. S1. The OH1 (top) /OH2 (bottom)-type hydroxyl TiO_2 surface structures of anatase (101) (left), rutile (110) (middle), and brookite (210) (right), and the active sites for the OER process are marked in the figure. Red, grey and white represent oxygen, titanium and hydrogen atoms, respectively.

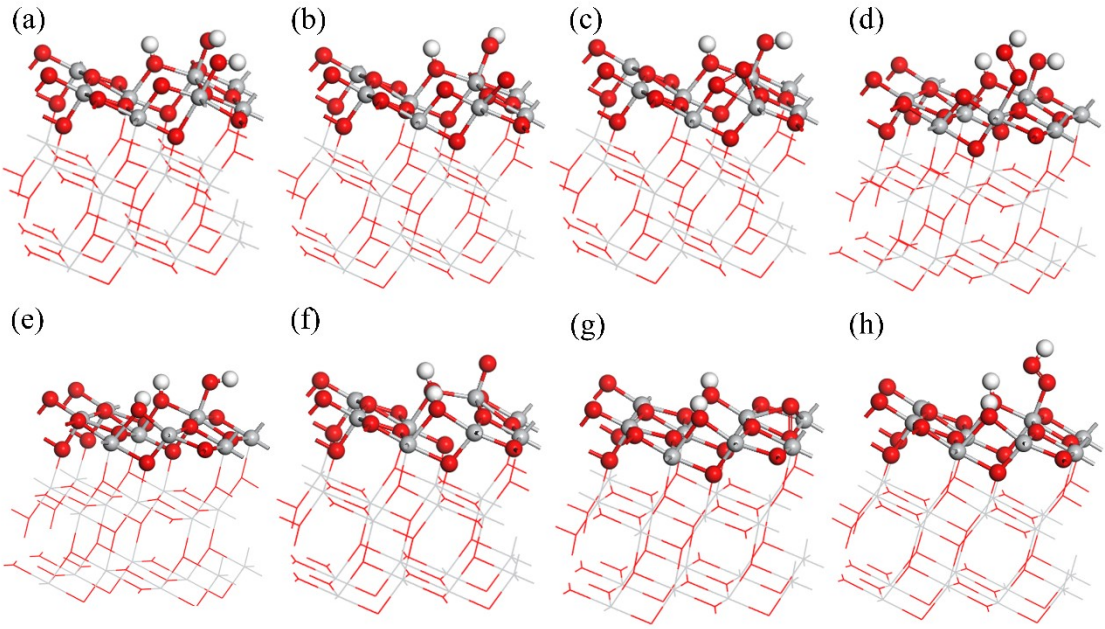

Fig. S2. The optimized structures of the adsorption intermediates of OH, Od, Op and OOH on A-101-OH1 (a-d) and A-101-OH2 (e-h) surfaces (side view).

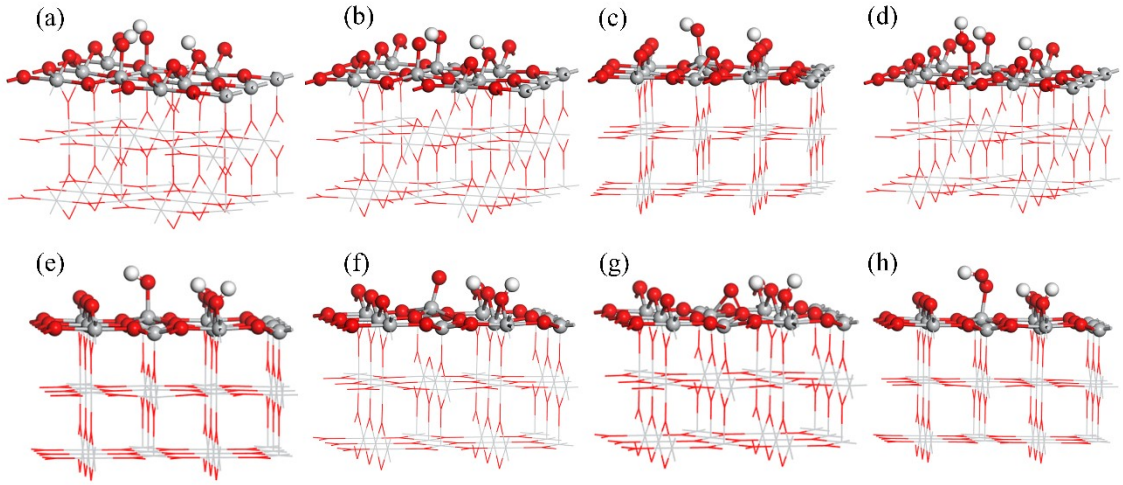

Fig. S3. The optimized structures of the adsorption intermediates of OH, Od, Op and OOH on R-110-OH1 (a-d) and R-110-OH2 (e-h) surfaces (side view).

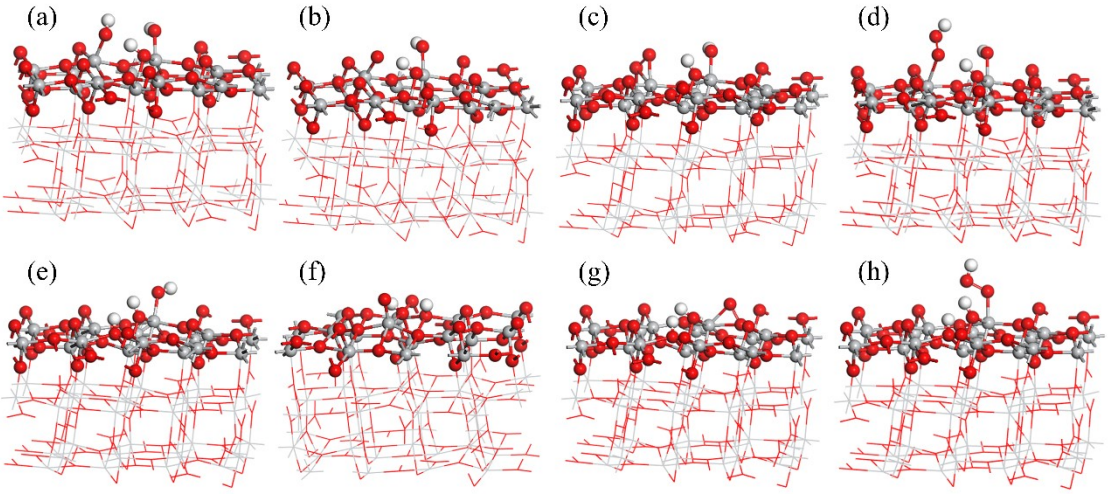

Fig. S4. The optimized structures of the adsorption intermediates of OH, Od, Op and OOH on B-210-OH1 (a-d) and B-210-OH2 (e-h) surfaces (side view).

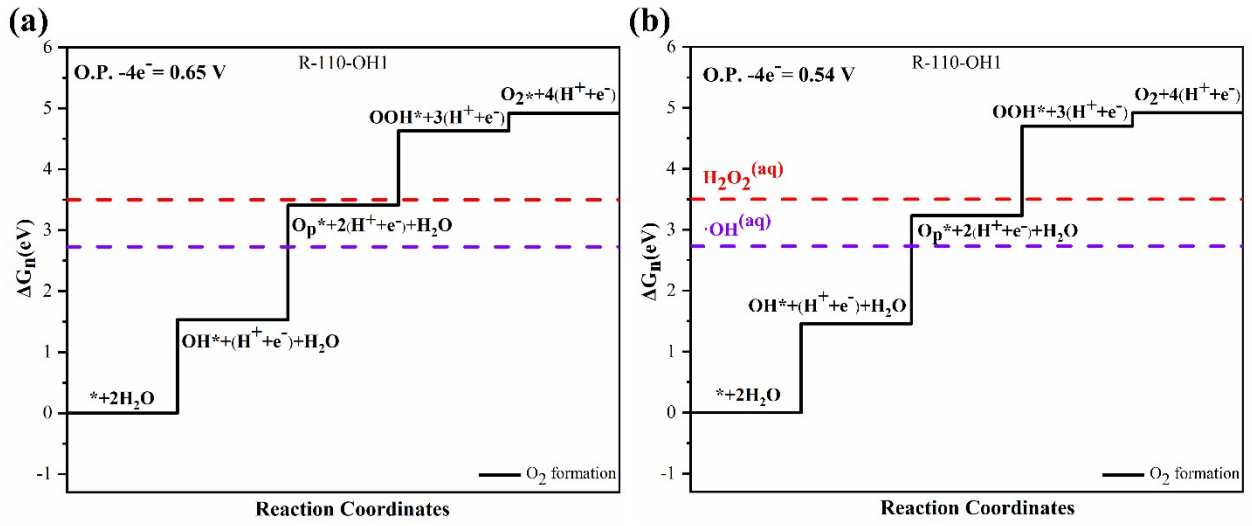

Fig. S5. The step free energy diagram of the oxygen evolution reaction process on the surface of R-110-OH1 calculated using the (a) GGA-PBE+U and (b) the GGA-PBE+D method.