

Supplementary Information for

**Hydrogenation of TiO₂ Nanosheets and Nanoparticles:
Typical Reduction Stages and Orientation-relative
Anisotropic Disordering**

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This PDF file includes:

Figure S1 to S5

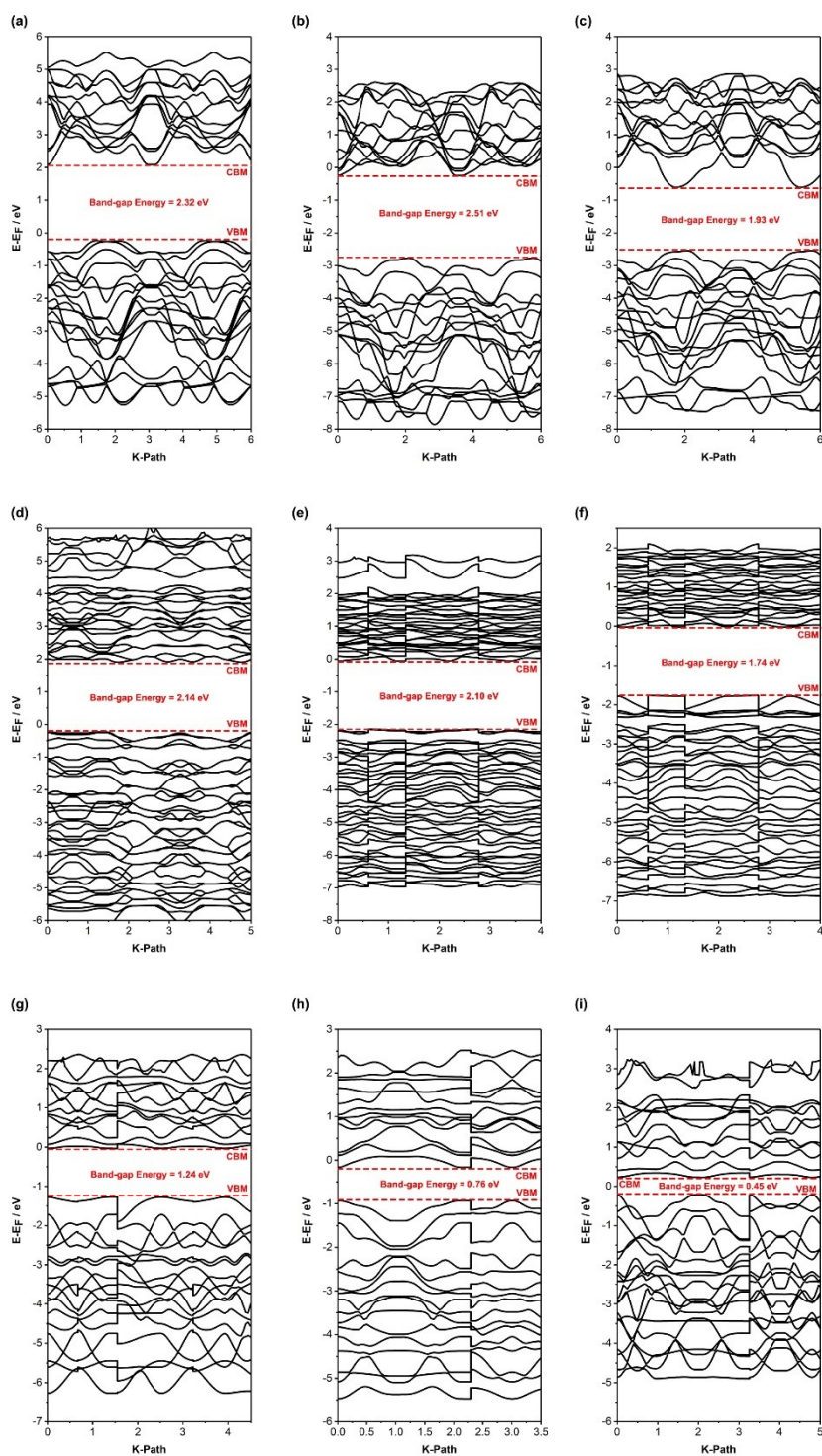


Figure S1 The energy band diagrams of (a) anatase, (b) anatase with $\text{H}/\text{O}_{2\text{C}}$, (c) anatase with $\text{H}/\text{O}_{3\text{C}}$. (d)(e)(f) denote the counterparts of brookite, and (g)(h)(i) denote the counterparts of rutile.

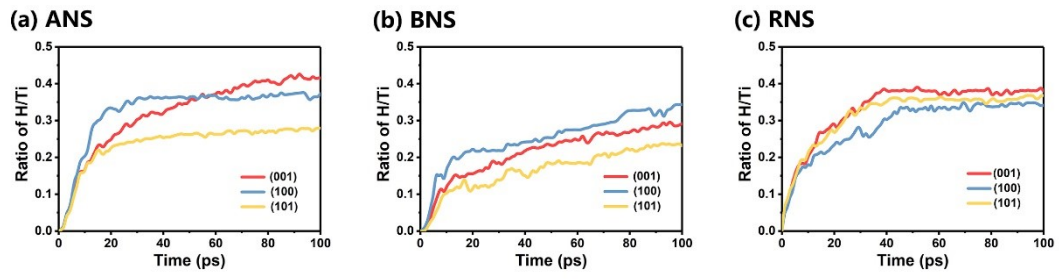


Figure S2 The variation of the ratio of H/Ti during the hydrogenation on the (001), (100), and (101) surfaces of the nanosheets.

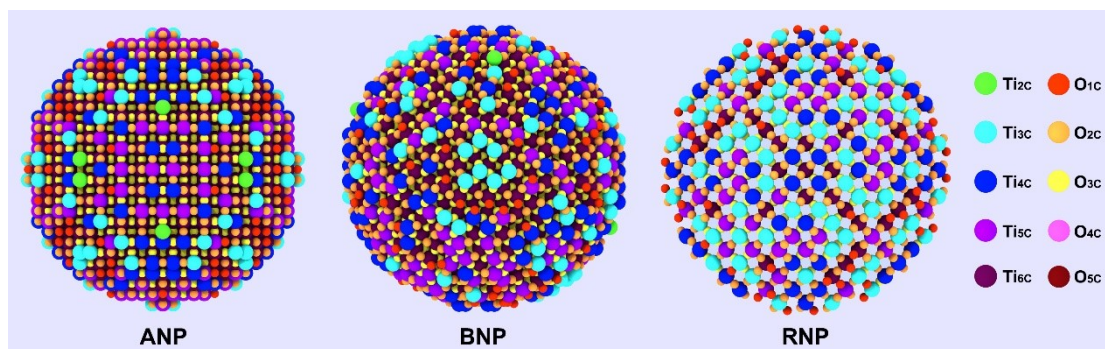


Figure S3 Atomic arrangement of the original modelling ANP, BNP and RNP surface. The surface atoms are painted into different colors according to their coordination numbers.

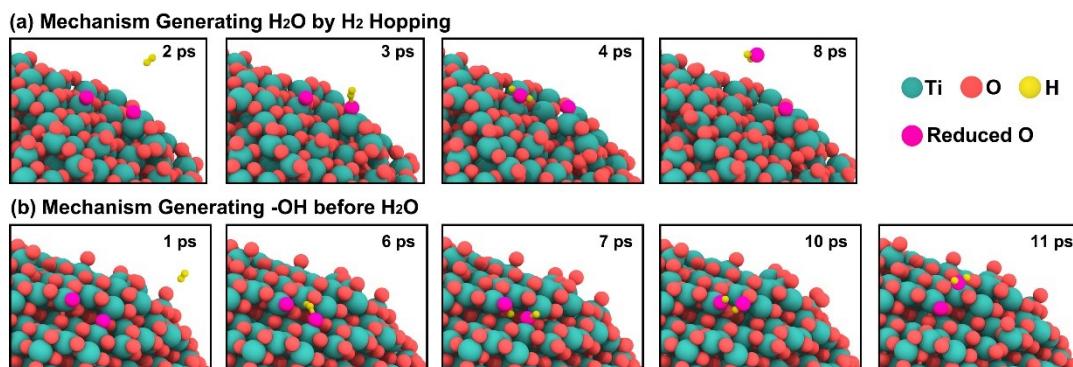


Figure S4 Two typical reduction mechanisms generating H₂O. Only partial atoms of the nanoparticles and H atoms participating the reduction are shown for distinct identification. The eventually reduced O atoms are colored pink.

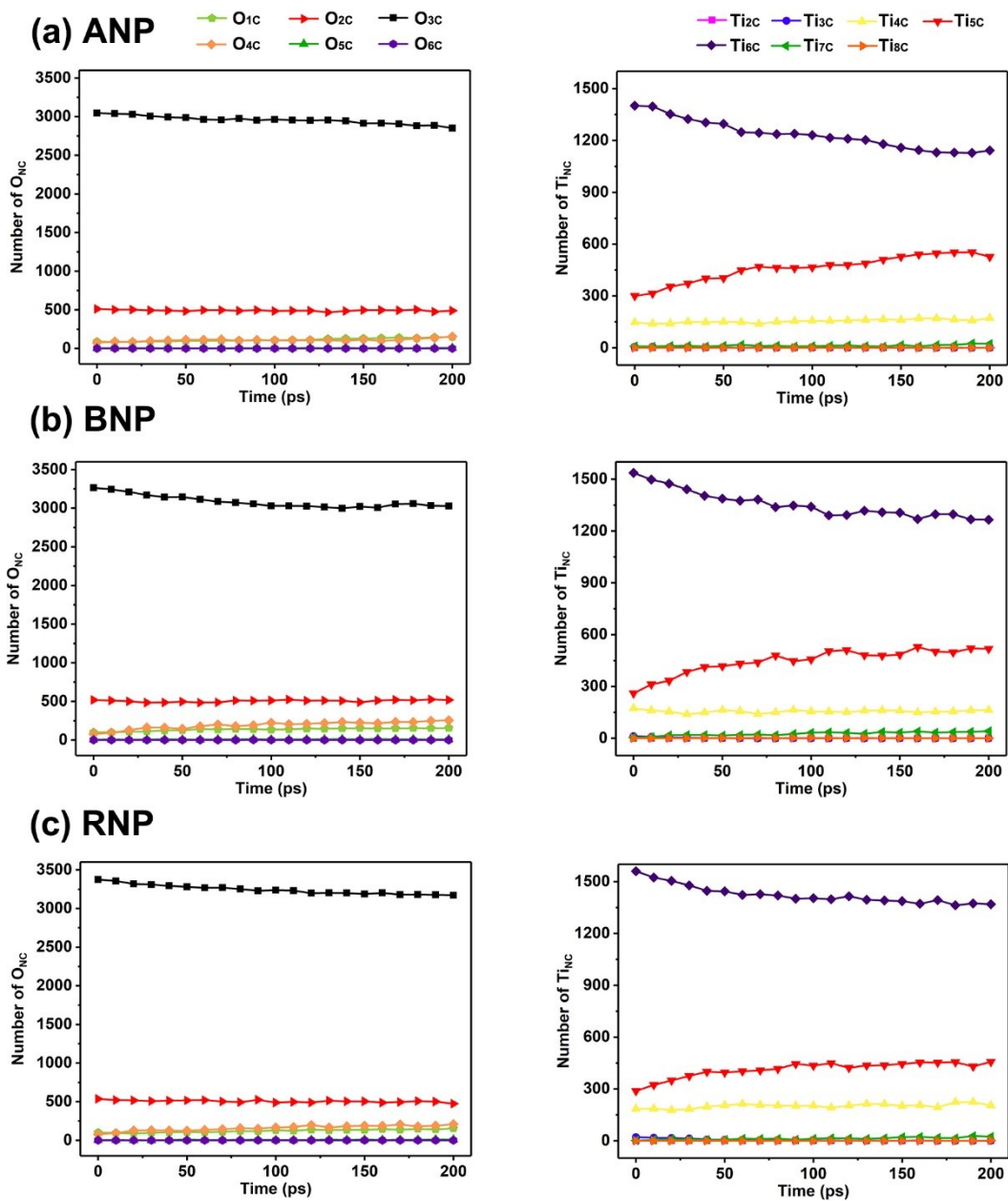


Figure S5 The variations of O_{NC} ($N = 1-6$), Ti_{NC} ($N = 2-8$) of (a) ANP, (b) BNP, (c) RNP during the reduction under the environmental setup of 1000 K, 200 atm and 4300 H_2 .