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Supporting Information

Stability of Adsorbed Water on TiO₂-TiN Interfaces. A First Principles and Ab Initio Thermodynamics Investigation

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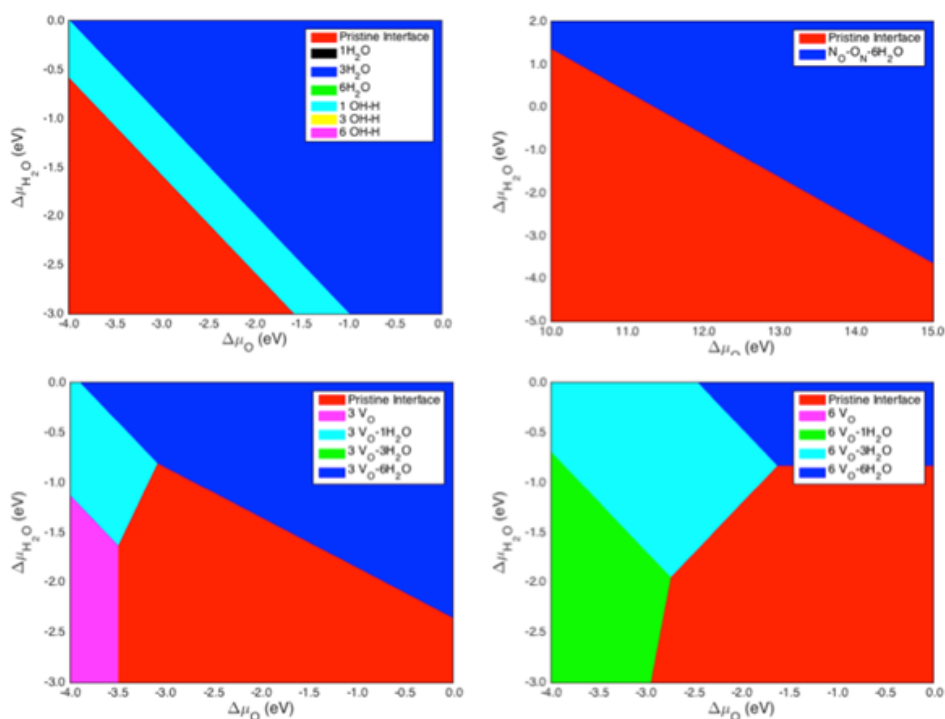


Figure S1. Surface phase diagrams of selected structures of TiN-TiO₂ in equilibrium with a ‘humid environment’, as a function of $\Delta\mu_{O_2}$ and $\Delta\mu_{H_2O}$ in the gas phase. Each diagram contains only selected structures and it shows their relative stability.

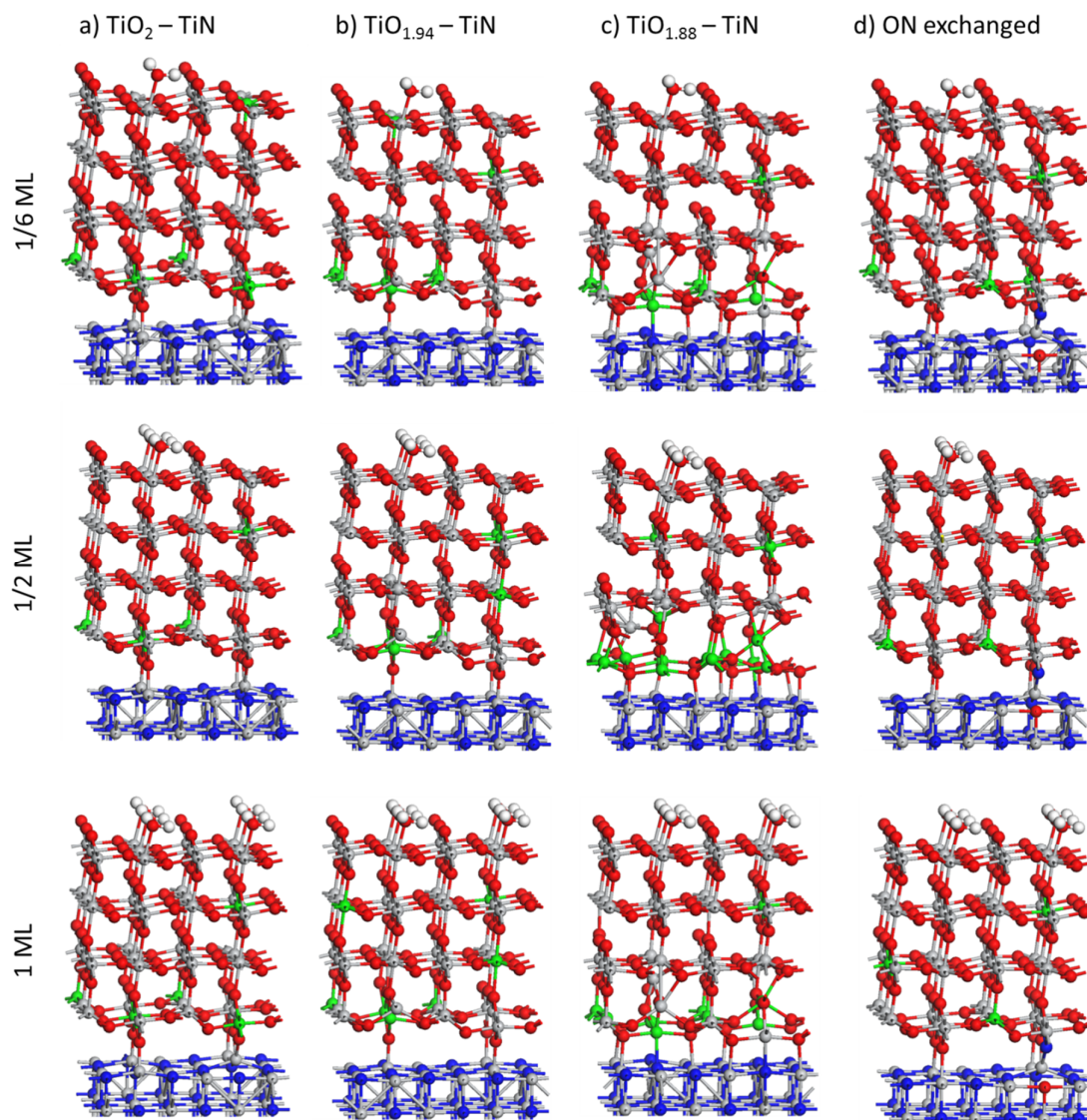


Figure S2. Structure of molecular water (H_2O) adsorbed on rutile TiO_2 (110)- TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2 - TiN , b) O defective $\text{TiO}_{1.94}$ - TiN , c) O defective $\text{TiO}_{1.88}$ - TiN and d) O/N exchanged TiO_2 - TiN interfaces. The rows from top to bottom are 1/6 ML (isolated water), 1/2 ML and 1 ML surface coverage ratios. The Ti^{3+} atoms in TiO_2 are represented by green spheres, Ti^{4+} atoms in TiO_2 and all Ti in TiN are grey, N atoms are blue, O atoms are red and H atoms are white.

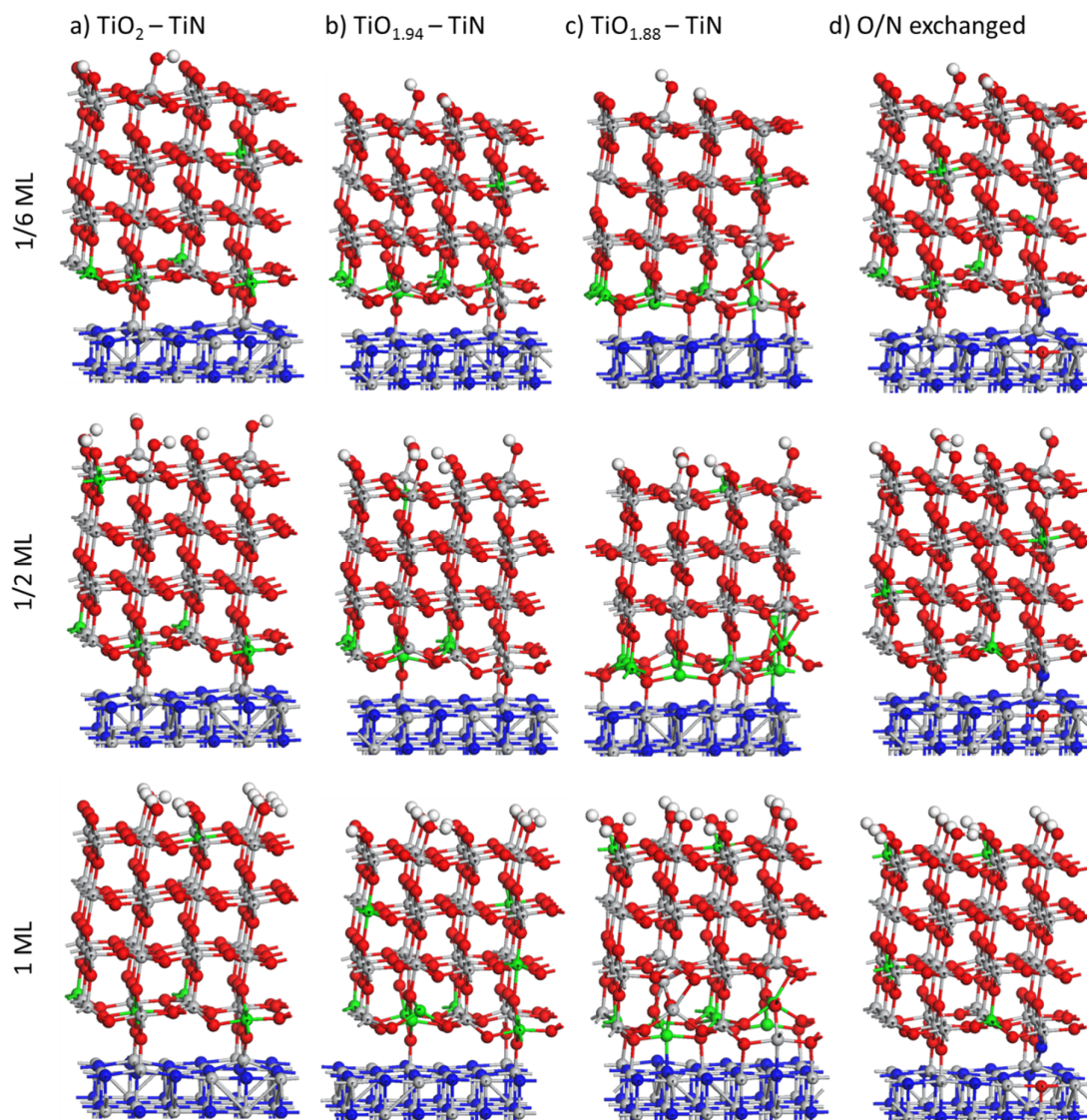


Figure S3. Structure of dissociated water (OH-H) adsorbed on rutile TiO_2 (110)-TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2 -TiN, b) O defective $\text{TiO}_{1.94}$ -TiN, c) O defective $\text{TiO}_{1.88}$ -TiN and d) O/N exchanged TiO_2 -TiN interfaces. The rows from top to bottom are for 1/6 ML (isolated water), 1/2 ML and 1 ML surface coverage ratios. The Ti^{3+} atoms in TiO_2 are represented by green spheres, Ti^{4+} atoms in TiO_2 and all Ti in TiN are grey, N atoms are blue, O atoms are red and H atoms are white.