Supporting Information

Stability of Adsorbed Water on TiO_2-TiN Interfaces. A First Principles and Ab Initio Thermodynamics Investigation

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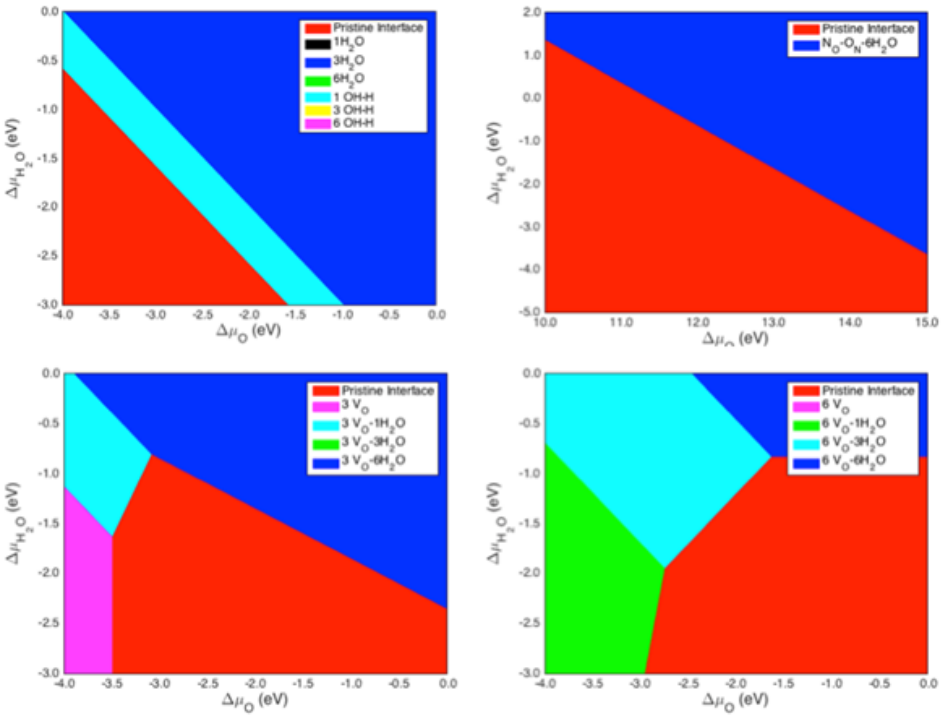

Figure S1. Surface phase diagrams of selected structures of TiN-TiO_2 in equilibrium with a ''humid environment'', as a function of $\Delta\mu_{O_2}$ and $\Delta\mu_{H_2O}$ in the gas phase. Each diagram contains only selected structures and it shows their relative stability.

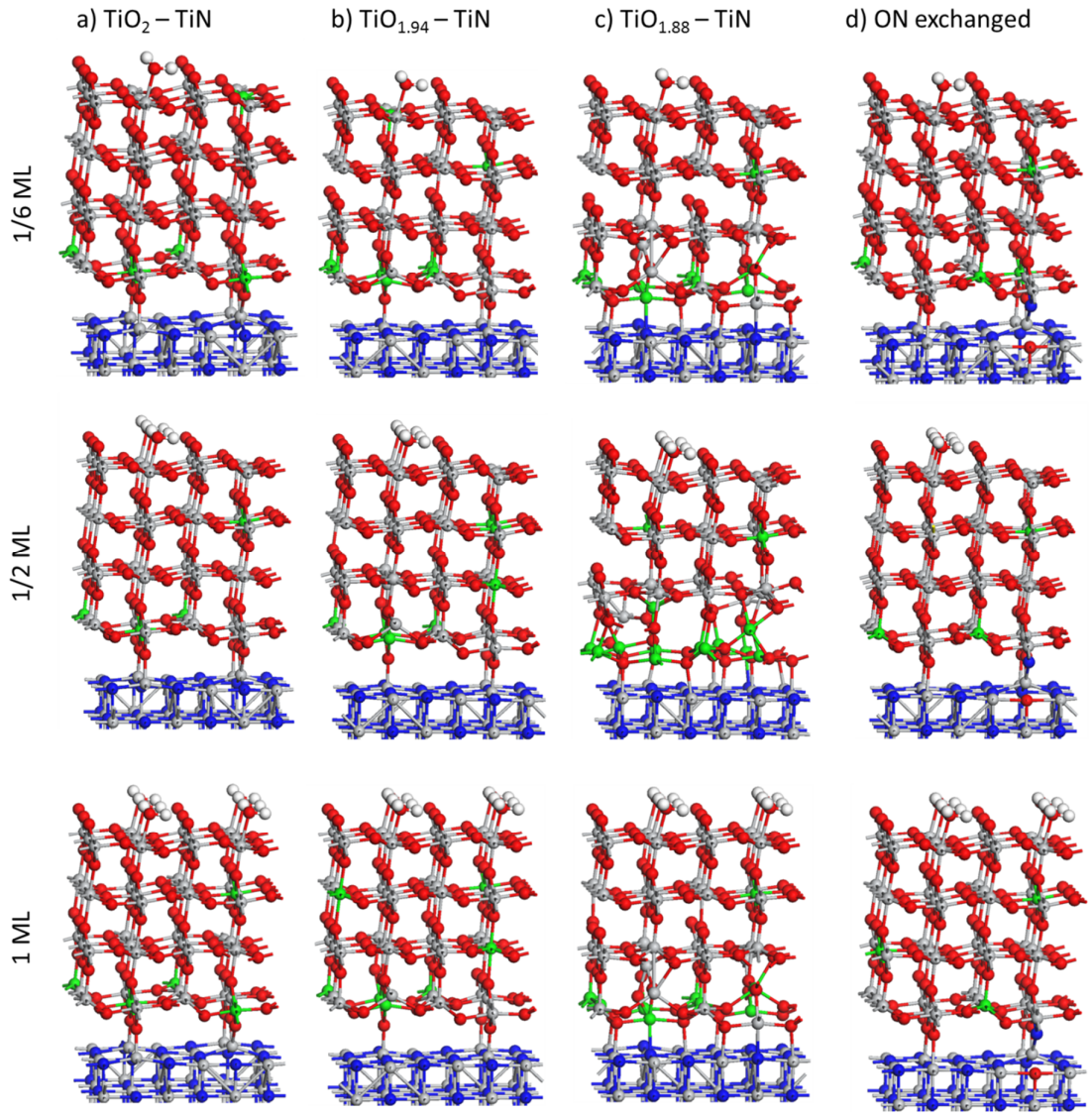

Figure S2. Structure of molecular water (H_2O) adsorbed on rutile TiO_2 (110)-TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2-TiN, b) O defective $TiO_{1.94}$-TiN, c) O defective $TiO_{1.88}$-TiN and d) O/N exchanged TiO_2-TiN interfaces. The rows from top to bottom 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.

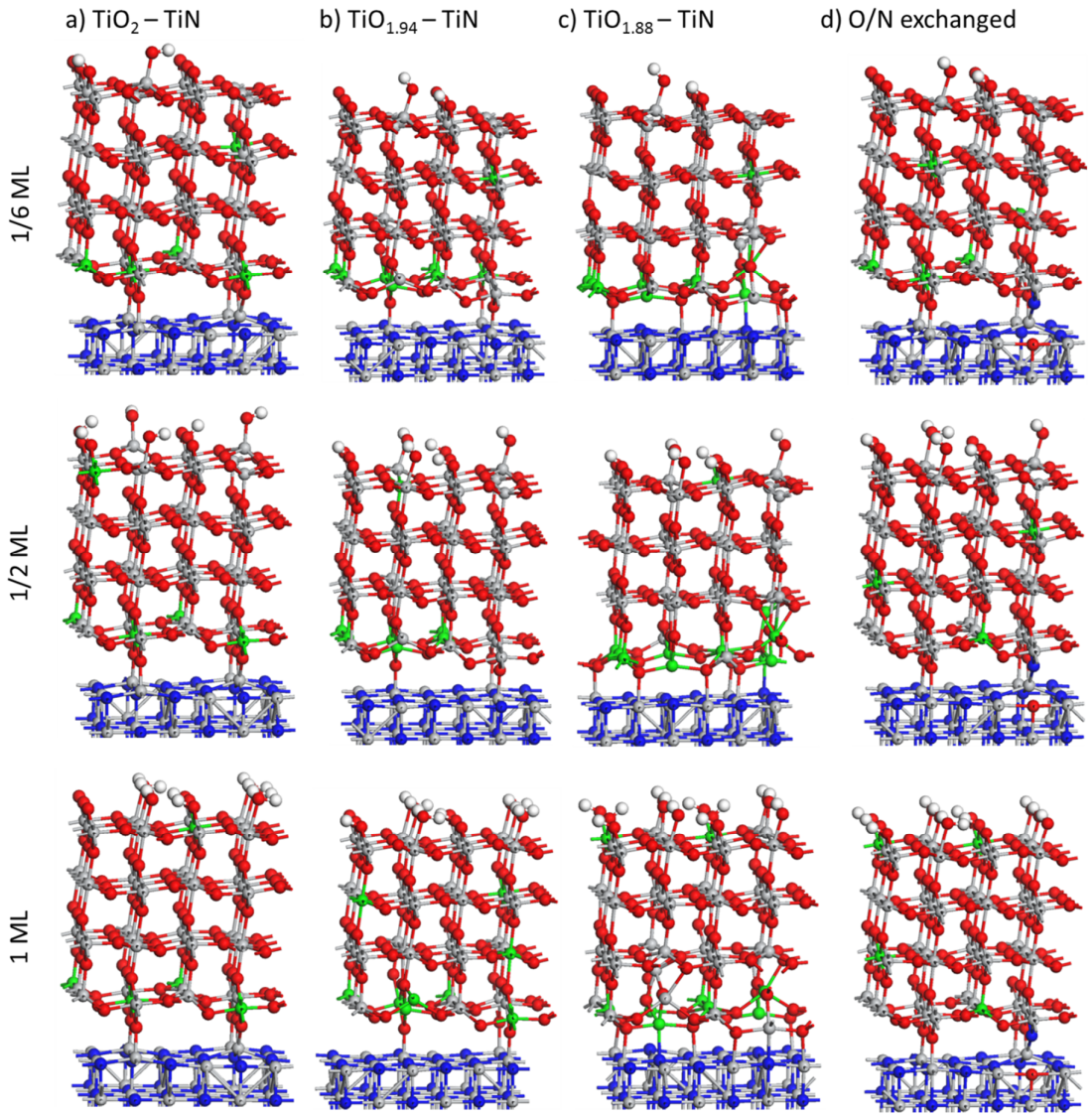

Figure S3. Structure of dissociated water (OH-H) adsorbed on rutile TiO_2 (110)-TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2-TiN, b) O defective $TiO_{1.94}$-TiN, c) O defective $TiO_{1.88}$-TiN and d) O/N exchanged TiO_2-TiN interfaces. The rows from top to bottom 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.