

Title	Stability of adsorbed water on TiO ₂ -TiN interfaces. A first-principles and ab initio thermodynamics investigation
Authors	Gutiérrez Moreno, José Julio; Fronzi, Marco; Lovera, Pierre; O'Riordan, Alan; Nolan, Michael
Publication date	2018-06-11
Original Citation	Gutiérrez Moreno, J. J., Fronzi, M., Lovera, P., O'Riordan, A. and Nolan, M. [2018] 'Stability of adsorbed water on TiO ₂ -TiN interfaces. A first-principles and ab initio thermodynamics investigation', Journal of Physical Chemistry C, 122(27), pp. 15395-15408. doi: 10.1021/acs.jpcc.8b03520
Type of publication	Article (peer-reviewed)
Link to publisher's version	10.1021/acs.jpcc.8b03520
Rights	© 2018, American Chemical Society. This document is the Accepted Manuscript version of a Published Work that appeared in final form in Journal of Physical Chemistry C, after technical editing by the publisher. To access the final edited and published work see: https://doi.org/10.1021/acs.jpcc.8b03520
Download date	2025-07-02 18:21:27
Item downloaded from	https://hdl.handle.net/10468/11770



UCC

University College Cork, Ireland
 Coláiste na hOllscoile Corcaigh

Supporting Information

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

José Julio Gutiérrez Moreno¹, Marco Fronzi², Pierre Lovera¹, Alan O’Riordan¹, Michael Nolan^{1*}

¹Tyndall National Institute, University College Cork. Lee Maltings, Dyke Parade. Cork, T12 R5CP, Ireland.

²International Research Centre for Renewable Energy, State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China.

michael.nolan@tyndall.ie

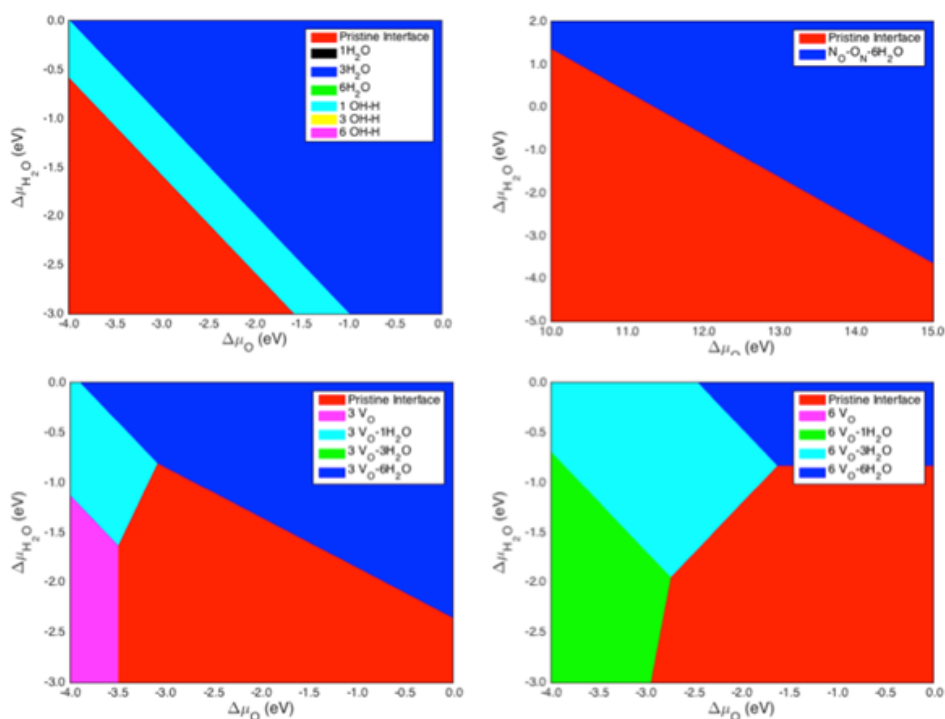


Figure S1. Surface phase diagrams of selected structures of TiN-TiO₂ in equilibrium with a ‘humid environment’, as a function of $\Delta\mu_{O_2}$ and $\Delta\mu_{H_2O}$ in the gas phase. Each diagram contains only selected structures and it shows their relative stability.

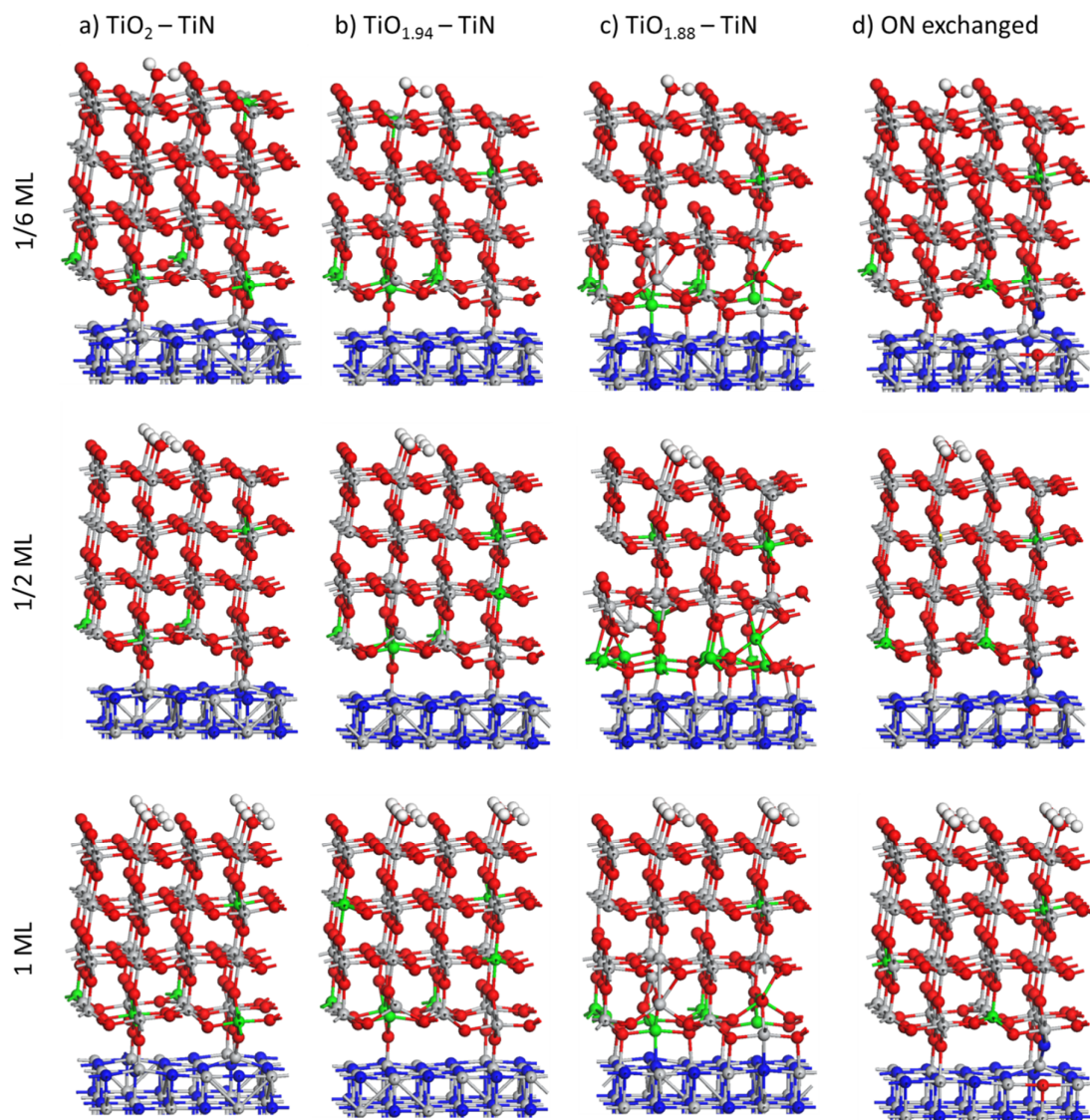


Figure S2. Structure of molecular water (H_2O) adsorbed on rutile TiO_2 (110)- TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2 - TiN , b) O defective $\text{TiO}_{1.94}$ - TiN , c) O defective $\text{TiO}_{1.88}$ - TiN and d) O/N exchanged TiO_2 - TiN interfaces.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

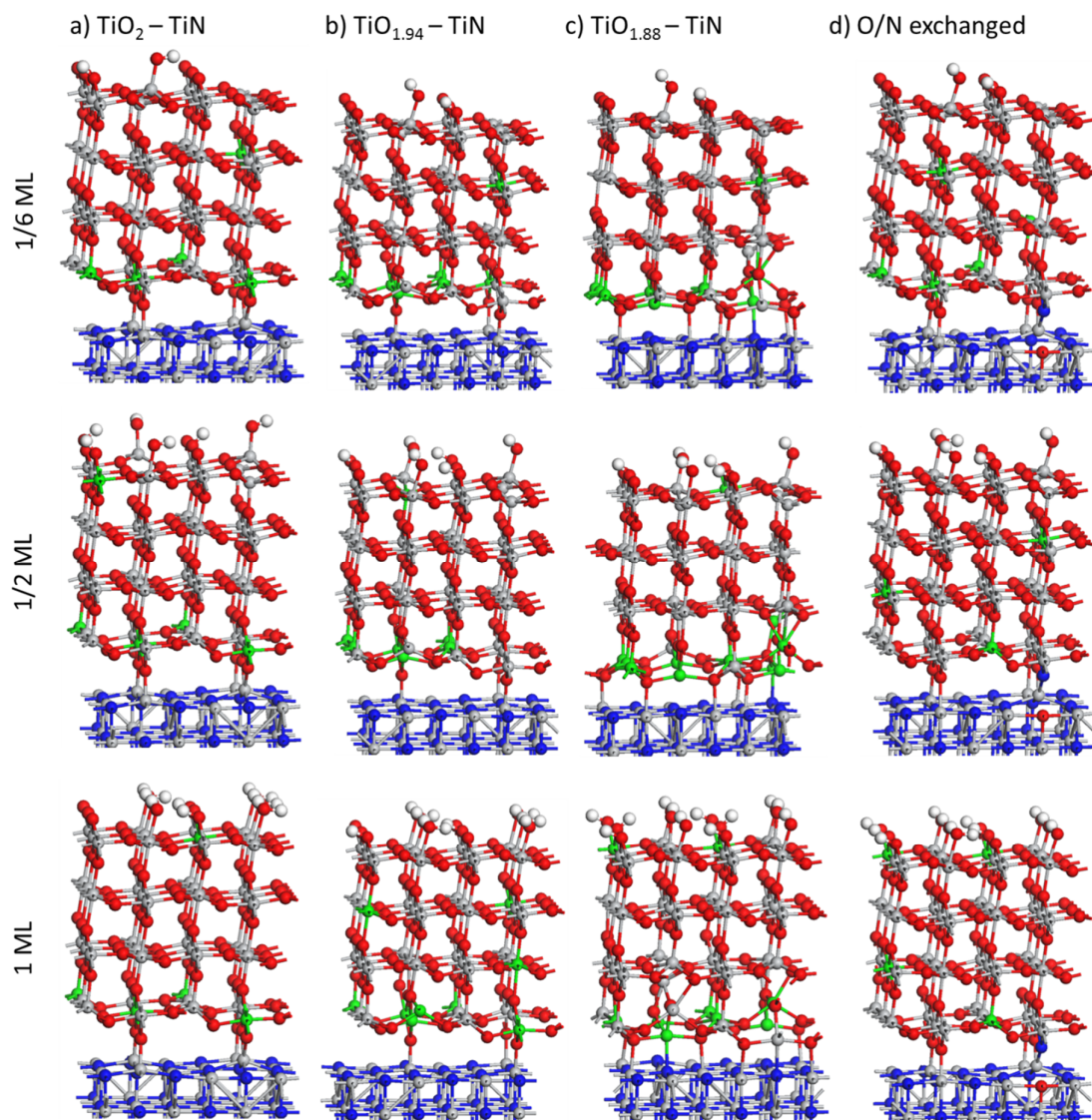


Figure S3. Structure of dissociated water (OH-H) adsorbed on rutile TiO_2 (110)-TiN (100) interfaces. Represented in columns from left to right are a) perfect TiO_2 -TiN, b) O defective $\text{TiO}_{1.94}$ -TiN, c) O defective $\text{TiO}_{1.88}$ -TiN and d) O/N exchanged TiO_2 -TiN interfaces. The rows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