

# Rutile TiO<sub>2</sub>(011)(2x1): Geometric Structure After Water Adsorption

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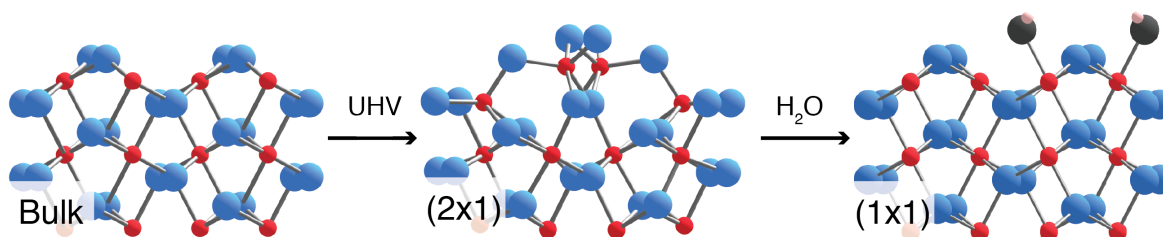
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Subsequent to the discovery that TiO<sub>2</sub> splits water into hydrogen and oxygen in a photoelectrochemical cell [1], there has been an immense drive to probe and enhance the photo-stimulated activity of TiO<sub>2</sub>. Effort has extended from synthesis and characterization of engineering materials (e.g. titania films) [2] to fundamental studies on model single crystal TiO<sub>2</sub> surfaces [3]. An essential component of this latter work is quantitative elucidation of surface geometric structure, without which full mechanistic understanding can never be realised. For example, structural investigations [4-6] have been applied to elucidate the surface structure of rutile-TiO<sub>2</sub>(011), as this surface is reported to display enhanced photo-catalytic activity [7]. The optimised structures emerging from these independent diffraction studies are essentially convergent, and so the surface structure has been reliably determined. Nevertheless, as yet, it remains unclear how the surface geometry of rutile-TiO<sub>2</sub>(011) results in enhanced photo-activity. One possible reason for the uncertainty surrounding the link between TiO<sub>2</sub>(011) surface structure and its photo-activity is that the surface probed by these investigations [4-6] is simply not pertinent, i.e. the photoactive surface phase exhibits a different termination.

Using surface X-ray diffraction, we have examined the UHV prepared rutile-TiO<sub>2</sub>(011)(2x1) surface after exposure to 20 mbar H<sub>2</sub>O. The surface exhibits a change in surface reconstruction – (2x1) to bulk-like (1x1) - driven by the formation of half a monolayer of hydroxyls at the interface.



## References:

- [1] K. Honda and A. Fujishima, *Nature* **238**, 37 (1972).
- [2] O. Carp *et al*, *Prog. Sol. State Chem.* **32**, 33 (2004).
- [3] U. Diebold, *Surf. Sci. Rep.* **48**, 53 (2003).
- [4] X. Torrelles *et al*, *Phys. Rev. Lett.* **101**, 185501 (2008).
- [5] X.-Q. Gong *et al*, *Surf. Sci.* **603**, 138 (2009).
- [6] S.E. Chamberlin *et al*, *Surf. Sci.* **603**, 3367 (2009).
- [7] T. Ohno *et al*, *New J. Chem.* **26**, 1167 (2002).