

## Charge transfer induced water splitting on the rutile TiO<sub>2</sub> (110) surface

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In direct contact with water, metal oxides are promising candidates in the search for renewable energy sources through direct photo-splitting of water as suggested by the seminal experiments of Fujishima and Honda [1]. TiO<sub>2</sub> is in particular one of the most utilized photo-chemically active systems for waste water treatment. For such photo-chemical processes, surface bound water as well as hydroxyls have been proposed to be the major species which are photo-activated to form hydroxyl radicals responsible for the photochemical activity.

By means of scanning tunneling microscopy (STM) we have identified a number of different water-derived adsorbates on the TiO<sub>2</sub>(110) surface, and the details of their formation were revealed from time-lapsed STM movies. We find strong evidence that the diffusion of hydroxyls, as well as H<sub>2</sub>O dissociation, is linked to the electronic properties of the substrate in the surface region, in a similar manner to our previous results reported for the interaction of O<sub>2</sub> molecules with TiO<sub>2</sub>(110) [2]. Hence, charge transfer from the conduction band of the substrate to adsorbed molecules or reactants is identified as a key factor to understand their physical properties. In other words, chemical reactions can be promoted, not only by a localized "active" site (the traditional approach), but also by the more delocalized conduction band electrons.

### References

- [1] A. Fujishima and K. Honda, *Nature* **37**, 238 (1972).
- [2] E. Wahlström *et al.*, *Science* **303**, 511 (2004).