

Water Dissociation on TiO₂ imaged by Atom-resolved Non-contact AFM

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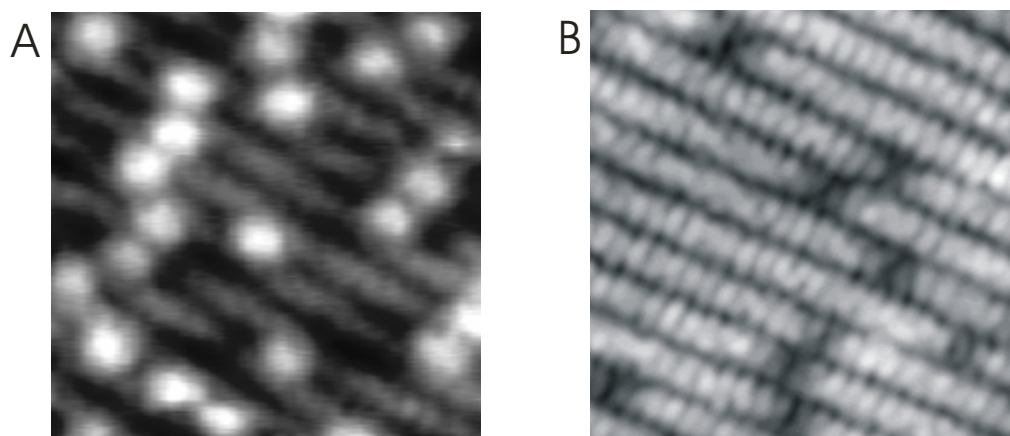
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Rutile TiO₂ has often served as a prototypical model system for the wealth of metal-oxides used in catalysis, and especially scanning probe techniques have in recent years given us very detailed insight into fundamental processes occurring on this oxide. Contrary to STM, where the contrast originates from a complex convolution of geometric and electronic structure, the atomic contrast in non-contact (or dynamic) AFM is often assumed to be primarily associated with geometric features. This is, however, not universally true since the atomic contrast is determined by the exact nature of the interaction forces between the surface and the tip [1].



In this study we show that adsorbed water on the surface *marks* the surface sublattices and by comparing with AFM simulations we can identify the tip polarity. This then allows us to obtain unprecedented atomic scale information on the structure and behaviour of dissociated water on the surface. Specifically, we find that two very different types of resolution with non-contact AFM are predominant on the hydroxylated TiO₂(110) surface. In one type of image contrast, the fivefold coordinated Ti rows are imaged as bright rows and the OH groups are visible as surprisingly bright protrusions located in between Ti rows (Figure 1A). Conversely, in the other predominant type of images the hydroxyls are imaged as slight 60 pm deep depressions in line with the rows of bridging oxygen atoms (Figure 1B). Clear atomic resolution was possible for the latter case which also shows that some holes occupy two sites. We tentatively interpret the double holes as two hydroxyls formed side-by-side by dissociation of water in an oxygen vacancy.

- [1] A. S. Foster, O. H. Pakarinen, J. M. Airaksinen, J.D. Gale and R. M. Nieminen, Phys. Rev. B 68 (2003) 195420