

# Atomic-scale structure and reactivity of the hematite $\alpha\text{-Fe}_2\text{O}_3$ (1-102) surface

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Hematite ( $\alpha\text{-Fe}_2\text{O}_3$ ) is a promising material for technological applications due to its abundance, low cost and chemical stability. Its 2.2 eV bandgap makes it potentially ideal as a photoanode for photoelectrochemical water splitting, but performance is hampered by slow reaction kinetics and the need for a significant overpotential. Little is known about the atomic-scale structure of hematite surfaces, and even less about how this relates to photocatalytic activity.

To date, most surface science studies of  $\alpha\text{-Fe}_2\text{O}_3$  have focused on the (0001) facet, but preparing a stoichiometric surface under UHV conditions has proven problematic. Some authors have investigated the equally relevant (1-102) surface, [1-3] and reported that a (1x1) and a reduced (2x1) termination can be reversibly prepared. Several models have been proposed for the (2x1) reconstruction, but as of now no scanning probe data exists to support or refute them.

Here we present an atomic-scale scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) study of the (1x1) and (2x1) surfaces of  $\alpha\text{-Fe}_2\text{O}_3$  (1-102). The data acquired for the (1x1) termination support a bulk termination model, as predicted by previous publications, but STM and nc-AFM images of the (2x1) reconstruction are inconsistent with previously proposed models. We propose a new model based on ordered oxygen vacancies, the plausibility of which is confirmed by density functional theory (DFT) results.

Both surfaces are active for the dissociative adsorption of water, the nature of which needs to be understood at an atomic scale in order to model catalytic reactions. We present results from a comprehensive study of this adsorption behaviour, based on STM, nc-AFM, x-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD).

## References:

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