

Abstract Submitted
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Adsorption and dissociation of water at the rutile TiO₂(011)-2x1 surface THOMAS BECK, MATTHIAS BATZILL, ANDREAS KLUST, ULRIKE DIEBOLD, Tulane University, CRISTIANA DI VALENTIN, Università degli Studi di Milano-Bicocca, ANTONIO TILOCCA, ANNABELLA SELONI, Princeton University — Surface science studies of rutile TiO₂ are increasing in popularity. There is evidence that TiO₂'s reactivity has strong dependencies of the reactivity on the surface orientation. Here studies on the (011) surface are presented and we demonstrate that this surface exhibits a higher activity towards the dissociation of water than the (110) surface. We recently demonstrated that the (011) reduces its energy by forming a 1x2 reconstruction.¹ This surface exhibits Ti=O (titanyl) groups that makes it unique compared to any other TiO₂ surface. Variable temperature UPS and room temperature STM together with molecular dynamics (MD) and DFT calculations have been employed to show that water dissociates at the perfect (011)-1x2 surface at temperatures below ~300 K, forming submonolayer coverage of hydroxyl groups. A mixed monolayer of dissociated and molecular adsorbed water is obtained below ~150 K. Water dissociating on the defect free (011) surface is in stark contrast to the (110) surface where dissociation is mediated by oxygen vacancies only. MD calculations indicate that the reduced distance between the H-atom of the adsorbed water and the surface oxygen atom at the (011) surface compared to the (110) surface facilitates dissociation. ¹ T.J. Beck et al. Phys. Rev. Lett. 93, 036104 (2004).

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