

## Surface defect-mediated reactivity of Au/TiO<sub>2</sub>(110)

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Metal clusters supported by transition metal oxides, as exemplified by the Au/TiO<sub>2</sub> system, have found broad applications as catalytic and sensor materials. The unusual properties of these systems originate from the specific interactions of metal clusters mediated by an oxide substrate, including local reduction below the cluster. In this work, we present recent results on the local interactions between one-dimensional defects on a TiO<sub>2</sub> surface and their reactivity with oxygen and Au nano-clusters studied by a combination of Scanning Tunneling Microscopy and Spectroscopy. High-resolution STM images, interpreted with first-principles theory, show that the observed one-dimensional strands have partially reduced Ti atoms coordinated at oxygen octahedral sites. When strands are exposed to  $5 \times 10^{-7}$  Torr O<sub>2</sub> at 300 K, oxygen is adsorbed and randomly nucleated on and along the strands. The results indicate the presence of exposed Ti ions that act as an active site for oxygen adsorption even at room temperature. Gold nano-particles of diameters 5 nm and less have also been deposited on the sub-stoichiometric rows of TiO<sub>x</sub> and characterized by STM. Like point defects and step edges on TiO<sub>2</sub>(110), the strands serve as nucleation sites for gold nano-clusters. The 1D defects of the surface are interpreted in terms of a surface crystallographic shear type structure, in contrast to the proposed Ti<sub>2</sub>O<sub>3</sub> added row model by Onish and Iwasawa [Phy. Rev. Lett. 76, (1996) 791]. The implications of this behavior and specific interaction between gold clusters, defects and gas molecules for catalytic activity of the Au/TiO<sub>2</sub> system are discussed.

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