Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Surface defect-promoted interaction of TiO_2(110) with molecular oxygen KEN PARK, Department of Physics, Baylor University, MINGHU PAN, Department of Physics and Astronomy, University of Tennessee, VINCENT MEUNIER, WILLIAM SHELTON, Computer Science and Mathematics Division, Oak Ridge National Laboratory, SERGEI KALININ, ARTHUR BADDORF, Condensed Matter Sciences Division, Oak Ridge National Laboratory, E.W. PLUMMER, Department of Physics and Astronomy, University of Tennessee — We present recent results on the local interactions between surface defects on a TiO_2(110) and their reactivity with oxygen 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 forming edge-sharing octahedra. When strands are exposed to 5 x 10^{-7} Torr O_2 at 300 K, oxygen is adsorbed and preferentially nucleated on and along the strands, indicating the presence of exposed Ti ions. The exposure to molecular oxygen also results in oxygen adsorption at Ti^{4+} sites on (1x1)-terminated terraces. The adsorbed oxygen species result in dark "defective"features in STM, identical to those on the pristine TiO_2(110), and further diffuse on the surface. The implications of this behavior and specific interaction between defects and gas molecules for catalytic activity are discussed.

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Date submitted: 15 Dec 2004 Electronic form version 1.4