

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Surface Reconstruction and Molecular Adsorption on Anatase $\text{TiO}_2(001)-(1\times 4)$ HUIJUAN SUN, YANG WANG, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science and Technology of China, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM — TiO_2 is a large band gap semiconductor with a wide range of applications including in photocatalysis, decontamination, and solar-energy conversion. Comparing to the well studied rutile phase, the anatase phase appears more common in nanocrystals and shows higher activity in photocatalysis. However, only a few literatures investigated the surface structure of anatase(001), which is assumed to be the origin of anatase's high reactivity, due to its thermodynamic instability and the difficulty in obtaining high quality samples. In the present work, reconstructed anatase $\text{TiO}_2(001)(1\times 4)$ surface has been investigated by atomic resolved STM together with the first-principles calculations. Two types of defects were found on the surface, which appear as dark spots and bright spots. The adsorption behavior of H_2O , O_2 and CO_2 molecules were studied. Surprisingly, it was found that all the molecules only adsorbed on the defect sites, which is against to the current understanding of the high activity of anatase (001) surface. Based on first-principles calculations we provide a new structure model of O saturated $\text{TiO}_2(001)(1\times 4)$ surface, which behaves inactive in photocatalysis.

Huijuan Sun
University of Science and Technology of China

Date submitted: 19 Dec 2012

Electronic form version 1.4