Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Characterization of Terminal Hydroxyl on TiO2(110) Surface QIJING ZHENG, HAO FENG, SHIJING TAN, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science & Technology of China, UNIVERSITY OF SCIENCE & TECHNOLOGY OF CHINA TEAM — TiO_2 is important in a wide variety of applications, among which is the water splitting and hydrogen production. However, as an important intermediate product of H_2O splitting, terminal hydroxyl has not been well studied. In the present work, we have used STM together with first-principles calculations to investigate the terminal hydroxyl, ie., the hydroxyl adsorbed on 5 coordinated Ti atom. At 77K the STM image shows a fuzziness feature, which is associated with a high conductance and a low conductance state in the I-V spectral. Based on the first-principles calculations, we assign this feature to proton hopping between bridge oxygen and terminal oxygen with a hopping barrier of 0.29 eV. The hopping rate under various applied biases and the current follow a power-law: $R \sim I^N$, which implies an inelastic electron tunneling process. Moreover, the hopping rate increased exponentially with increasing biases, reminiscent of thermal excited Arrhenius relation, while in our case it is hot electron excitation.

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Date submitted: 13 Nov 2012 Electronic form version 1.4