Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Propane-1,3-diol Adsorption and Dissociation on Rutile TiO_2(110): A Scanning Tunneling Microscopy Study ZHENRONG ZHANG, Department of Physics, Baylor University, XIAO LIN, BRUCE KAY, ZDENEK DOHNÁLEK, Chemical and Materials Sciences Division, Fundamental and Computational Sciences Directorate, Pacific Northwest National Laboratory — Titanium Dioxide (TiO_2) has attracted great attention in the past decades due to its importance in heterogeneous catalysis. Here the adsorption and dissociation of Propane-1,3-diol molecules on partially reduced rutile TiO_2(110) surfaces are studied via variable temperature scanning tunneling microscopy (VT-STM). STM images of TiO_2(110) surfaces obtained before and after *in-situ* doses of melecules at room temperature show that the molecules preferentially bind in bridge-bonded oxygen vancanies (BBO_V's) *via* one O-H bond scission. The dynamics of Propane-1,3-diol molecules motion has been investigated at room and elevated temperatures. Propane-1,3-diol molecules swing on TiO_2 surface with one end (-CH_2-O^-) anchored on vacancies. Strong interaction of the other end (-O-H) with Ti_{5c} reduces the swing rate when compared with octanol.

Zhenrong Zhang
Department of Physics, Baylor University,
One Bear Place 97316, Waco, TX 76798-7316

Date submitted: 27 Nov 2010 Electronic form version 1.4