Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Photooxidation of sugar and alcohol on TiO_2 surfaces: A first-pirnciples study MAO-HUA DU, JUN FENG, SHENGBAI ZHANG, National Renewable Energy Laboratory — First-principles studies are carried out on TiO_2/sugar (alcohol) interfaces under UV illumination. A rapid charge separation takes place at the interfaces through a two-step process: (1) trapping of photo-generated carriers at the gap levels induced by the chemisorbed molecules, and (2) upon the carrier trapping, a structural transformation of the adsorbed molecules, which in turn eliminates the gap levels. The second-step here is necessary to avoid carrier recombination, and hence results in an irreversible charge separation. Such a charge transfer across the semiconductor/molecule interface leads to various oxidation and reduction processes with structural reconfigurations (bond- forming and breaking) of the surface molecules. These results reveal the underlying microscopic mechanism of photo-catalytic reactions on the TiO_2 surfaces. The mechanism for the observed self-assembly of TiO2/cyclodextrin wires under UV illumination will also be discussed. This work was supported by the U. S. Department of Energy, BES and EERE, under Contract No. DE-AC39-98-GO10337.

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Date submitted: 29 Nov 2005 Electronic form version 1.4