Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Water dissociation on TiO_2(110): application of the reactivity mapping method JORGE SOFO, Department of Physics and Materials Research Institute, Penn State, ELAM LEED, Department of Materials Science and Engineering, Penn State — We have recently developed a method to calculate the chemical reactivity of a surface with respect to water dissociation. The method is based on one calculation of the electronic states and provides a map of the activity of different sites at the surface. We present an application to the water physisorption and chemisorption process on the (110) surface of TiO_2 in the rutile structure. The predictions of this chemical reactivity mapping method are in excellent agreement with more conventional method of calculation chemical reactivity, including ab-initio molecular dynamics. As a result of its simplicity it is possible to study larger surface areas including the effect of correlations and catalytic effects.

Jorge Sofo
Department of Physics and Materials Research Institute, Penn State

Date submitted: 06 Dec 2004 Electronic form version 1.4