

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Simulation study of water/silicon oxide interface** CHRISTIAN LORENZ, SUSAN REMPE, MARK STEVENS, GARY GREY, Sandia National Laboratories, MESFIN TSIGE, Southern Illinois University — The interaction of water with solid surfaces plays a crucial role in many phenomena. The water-silica interface is one of the typical systems encountered in technological and natural materials. Numerous technological applications of silica were found to rely on its specific surface properties. Large scale quantum mechanics (QM) and classical molecular dynamics (MD) simulations are used to study the molecular configurations and wetting properties of water at the interface of different silicon oxide surfaces. In order to understand how the surface coverage of silanols (-SiOH) affects the wetting behavior of the silica surfaces, both crystalline ((001)  $\alpha$ -quartz (coverage  $9.6 \text{ nm}^{-2}$ ) and (100)  $\beta$ -cristobalite ( $7.8 \text{ nm}^{-2}$ )) and amorphous silica ( $5.0 \text{ nm}^{-2}$ ) substrates have been studied. The binding energy of the water, the number of water molecules hydrogen-bonded to the surface and the configuration of the hydrogen-bonded water molecules are determined as a function of silanol coverage from QM simulations. The number of water molecules within a monolayer and the orientation of the water molecules within the monolayer and in the bulk are determined from MD simulations. Results from two classical force fields are compared to one another and to the relevant quantities from the QM simulations. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 30 Nov 2005

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