

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Hydrogen bond density and strength analysis on hydrated Rutile (110) and Cassiterite (110) surfaces NITIN KUMAR, Department of Physics, Penn State University, PAUL KENT, Center for Nanophase Materials Sciences and Chemical Sciences Division, Oak Ridge National Laboratory, ANDREI BANDURA, St. Petersburg State University, DAVID WESOLOWSKI, Chemical Sciences Division, Oak Ridge National Laboratory, JAMES KUBICKI, Department of Geosciences, Penn State University, JORGE SOFO, Department of Physics, Penn State University — We study the dynamics of water on the surface of cassiterite (110) and rutile (110) using ab-initio molecular dynamics simulation. Water adsorbs and dissociates on these surfaces. This dynamic equilibrium is dominated by the hydrogen bond (h-bond) network at the surface. The h-bond density analysis shows that adsorbed water molecules form higher average number of h-bonds on rutile (~ 2.3) as compared to the cassiterite surface (~ 2.1). On the other hand, bridging oxygen atoms form higher average number of h-bonds on cassiterite (~ 1.4) than rutile surface (~ 1.2). Dissociated species are found to have same average number of hydrogen bonds on both surfaces. As a consequence, the rutile surface has higher density of h-bonds at the surface than cassiterite, however, their strength is lower [N. Kumar et al., *J. Chem. Phys.* 134, 044706 (2011)]. This delicate balance is responsible for the different dynamical properties of both surfaces.

Nitin Kumar
Department of Physics, Penn State University

Date submitted: 11 Nov 2011

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