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Surface metal-oxygen bond length on hydrated rutile(110) and cassiterite(110) surface - A measure of the local environment 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 rutile (110) and cassiterite (110) using ab-initio molecular dynamics simulation. The water molecule covalently attach with the fivefold coordinated metal atoms on the surface. It can remain in a molecular form or it can dissociate to form hydroxyls on the surface. The distance between the metal and the oxygen depends on the protonation state of the latter. Moreover, we find that the local environment is not only limited to the number of covalently bonded hydrogen but it also depends on number of hydrogen bonds and the species participating in it. In general, the metal oxygen distance shows much larger fluctuations in rutile compared with cassiterite. The half width half maximum (HWHM) of the metal oxygen distance histogram, for the terminal oxygen, is 0.27 Angstrom for rutile and 0.16 Angstrom for cassiterite. Also, for bridging oxygen HWHM is 0.18 and 0.12 Angstrom for rutile and cassiterite, respectively.

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