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Ti-O bond distance fluctuations at the hydrated rutile (110) surface NITIN KUMAR, Department Of Physics, Penn State University, PAUL KENT, ORNL, DAVID COLE, DAVID WESOLOWSKI, Chemical Sciences Division, ORNL, JAMES KUBICKI, Department of Geosciences, The Pennsylvania State University, JORGE SOFO, Department of Physics, The Pennsylvania State University — We studied water on the rutile (110) surface using ab-initio molecular dynamics simulations in NVT ensemble at 280K, 300K, and 320K. Water adsorbs on the 5-fold coordinated titanium atoms or dissociates transferring a proton to a bridging-oxygen atom. The equilibrium between these configurations is dynamical and depends on temperature and water coverage. The titanium-oxygen bond distances at the surface can change as much as 12% depending on the number of hydrogen atoms bonded to oxygen. Hydrogen bonds also affect this distance. A measurement of the Ti-O distance at the surface can be used to estimate the average degree of dissociation. In view of our simulation results, the experimental evidence, such as photoelectron diffraction, indicates a low degree of dissociation under dry conditions.

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