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Hydrogen Bonds and the Vibrational Modes of Water at Interfaces: ab-initio Molecular Dynamics meets Neutron Scattering NITIN KUMAR, SANGHAMITRA NEOGI, Department of Physics, Penn State University, PAUL KENT, Oak Ridge National Laboratory, ANDREI BANDURA, Saint Petersburg State University, JAMES KUBICKI, Department of Geosciences, Penn State University, DAVID WESOLOWSKI, Oak Ridge National Laboratory, JORGE SOFO, Department of Physics, Penn State University — We study the vibrational density of states (VDOS) of a thin water layer on the rutile (110) surface. The VDOS is obtained from the velocity-velocity autocorrelation function calculated from trajectories of large scale ab-initio molecular dynamics simulations. The rutile surface induces a shift to lower frequencies of the stretching modes with respect to pure water. The water vapor surface shows a peak at the vibrational frequency of free hydroxyls. Overall, the average stretching mode vibrational frequency increases with decreasing hydrogen bonding density. This density depends strongly on temperature. The water dissociation percentage at the surface can be correlated with the ratio between the weights of the stretching and the bending modes. Our results are in good agreement with inelastic neutron scattering measurements done on wet titania nanoparticles.

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