

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effect of Ions and pH on the H-bond Network at the Quartz(101)-Water Interface¹ MARK DELLOSTRITTO, JAMES KUBICKI, JORGE SOFO, The Pennsylvania State University — Reactions in aqueous systems are common, and yet can be difficult to study, as the structure and dynamics of the H-bond network can dominate the rates of reactions by determining the access reactants have to each other. This is thought to be the case at the quartz-water interface, where the addition of ions to solution or an increase in pH can increase the dissolution rate by an order of magnitude without any change in the activation energy. This suggests that the dissolution reaction is unchanged and the ions modify the structure of water at the interface such that the reaction occurs at a greater frequency. To investigate this effect, we performed ab-initio molecular dynamics (AIMD) simulations of the quartz(101)-water interface in several different ionic solutions under different pH and temperature conditions. We found that both anions and cations in a near-surface configuration tend to increase the order of interfacial water, although at neutral pH this competes with a decrease in the H-bond lifetime induced by the presence of an anion-cation pair. We also found that neither the H or O atoms of H₂O or OH⁻ have greater access to the surface with the introduction of ions, but there is a greater incidence of intrasurface H-bonding in all systems studied. This suggests that intrasurface proton transfer could be an important component of the dissolution reaction, while nucleophilic attack of Si by H₂O is unlikely to occur at the interface studied.

¹Work supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences, U.S. Department of Energy

Mark DelloStritto
The Pennsylvania State University

Date submitted: 14 Nov 2014

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