Abstract Submitted
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**Detecting the Presence of Quartz-Dissolution Precursors with DFT-based Molecular Dynamics**[1] MARK DELLOSTRITTO, JORGE SOFO, Department of Physics, The Pennsylvania State University, State College, PA, JAMES KUBICKI, Department of Geosciences and the Earth and Environmental Systems Institute, The Pennsylvania State University, State College, PA — The study of water/oxide interfaces presents challenges as a result of the low symmetry of the system, the highly structured nature of water, and the difficulty of accurately modelling H-bond interactions. An example is the quartz-water interface, where adding ions to solution increases the dissolution rate by an order of magnitude, but without any change in the activation energy. This suggests that the ions alter the interfacial structure such that the dissolution reaction configuration becomes more accessible to the reactants, thereby decreasing the entropic barrier and increasing the rate of reaction. As the interfacial structure and dissolution reaction are dominated by H-bonding and proton transfer, DFT calculations are useful for simulating the interfacial configuration. We use DFT molecular dynamics simulations of the quartz-water interface with statistical measures of the interfacial structure and vibrational analysis to test whether or not ion-induced stable configurations increase the population of dissolution precursor states. We find that intrasurface proton transfer is likely to be a common precursor when an ion is near the surface, and that both direct proton transfer to the surface and nucleophilic attack of Si by $H_2O$ are unlikely to be reaction precursors.

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Mark DelloStritto
Dept of Physics, The Pennsylvania State University, State College, PA

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