Effects of Density and Temperature on the Adsorption of Molecular Water on Metallic Surfaces: a Molecular Dynamics Study

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A microscopic picture of water adsorption on metallic surfaces is relevant to several areas such as electrochemistry, catalysis and corrosion studies. In particular, very little is known about the mechanisms of corrosion at elevated temperatures and pressures, such as those required in new technologies for oxidation of toxic wastes. A detailed molecular level description is needed to help in the understanding of the problem and to provide firm guidelines for the design of experiments.

Here we use molecular dynamics (MD) simulations to characterize structural and dynamical properties of water adsorbed on Ni (111). The force fields to describe the water-Ni interactions are obtained using quantum density functional theory. The SPC/E model is used for water-water interactions. Post-processing of the simulation data is handled by standard methods of analysis such as determination of pair energy and density distribution functions and time correlation functions. The effects of increase in temperature and decrease in density on the adsorption properties and the influence of these variables on the disruption of the H-bond network are investigated. Both a clean surface and one precovered with oxygen are tested. Differences in orientations and structure of water as a function of the distance from the surface are discussed.