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dynamics of water at the 100 and 111 surfaces of platinum electrodes ADAM WILLARD, DAVID CHANDLER, University of California, Berkeley, PAUL MADDEN, University of Oxford — The results of molecular dynamics simulations of water in a model electrochemical cell is described. The model consists of water contained between two platinum electrodes that are polarizable and capable of being held at constant potential relative to the vacuum. The structure and fluctuations of water molecules adjacent to both the 100 and the 111 surfaces of a solid platinum electrode are considered. It is shown that the orientational distributions as well as the relaxation dynamics of the electrode-adsorbed water molecules depend significantly on electrode geometry. This dependence reflects competition between hydrogen bonding and non-hydrogen bonding interactions of electrode adsorbed water molecules, and whether electrode lattice geometry is commensurate with two-dimensional hydrogen bonding patterns of water. Furthermore the dynamics of adsorbed water molecules are spatially and temporally heterogeneous leading to slow reorganization of the hydrogen bond patterns adjacent to the metal surfaces.

Adam Willard
University of California, Berkeley

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