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Catalytic Mechanism Modeling of Oxygen/Platinum Systems using ReaxFF MD Simulation PAOLO VALENTINI, THOMAS SCHWARTZENTRUBER, University of Minnesota, IOANA COZMUTA, Eloret Corporation — ReaxFF Molecular Dynamics simulations are performed to study some of the fundamental surface mechanisms that characterize the catalytic behavior of a Pt(111) surface exposed to oxygen. The use of the reactive empirical potential ReaxFF allows the simulation of chemical bond breaking/formation, essential to describe the detailed processes at the surface, while maintaining computational feasibility for rather massive systems (thousands of atoms). The ReaxFF potential was initially trained using a set of Quantum Chemistry energy data relevant for the system of interest, including molecular/atomic adsorption enthalpies at various surface sites. Subsequently, the sticking coefficients were determined for oxygen molecules impinging onto the surface. The MD simulations well reproduce some of the experimental trends observed for the adsorption process in molecular-oxygen/platinum systems. At very low incident energies (less than 0.1 eV), the adsorption is determined by a weakly-bound physisorption state, but is rapidly suppressed by additional rotational energy (due to steric hindrance) or by increasing the substrate temperature. At higher incident energies, the sticking probability levels off due to dynamic trapping as observed experimentally. Because ReaxFF is solely based on Quantum Chemistry, the objective of this study is to extend the approach proposed here to other gas/surface systems for which good experimental evidence on the detailed catalytic surface processes is currently not available.

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