Platinum electrocatalysts for oxygen reduction: Theoretical studies

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Density functional theory (DFT), as well as classical molecular dynamics (MD) simulations and other statistical mechanical techniques are used for implementing a multi-scale modeling approach applied to the electroreduction of oxygen on platinum. We are interested in the description of the system cathode/electrolyte in proton-exchange membrane (PEM) fuel cells.

We characterize adsorption energies, molecular precursors for oxygen dissociation, and activation barriers for dissociation. The proton reaction with adsorbed atomic oxygen is analyzed using DFT methods, including solvent effects, whereas a combination of DFT and MD is used to analyze the proton transfer and interactions with a polymer electrolyte membrane. Finally, an effective Hamiltonian model1 is used to determine the interplay between the microscopic variables and the macroscopic effects, such as the effect of the overpotential on the activation barrier for electroreduction.

1M. T. M. Koper and G. A. Voth, J. Chem. Phys., 109, 1991-2001, (1998).