The mechanism of oxygen electroreduction on Pt(111)

P. B. Balbuena, Y. Wang and S. R. Calvo
Department of Chemical Engineering
Texas A&M University
College Station, TX 78743

Ab initio molecular dynamics simulations have been used to investigate the four-electron oxygen electroreduction on Pt(111) in acid medium. Our study includes the coupling of electron and proton transfer and the solvent and electrode potential effects.

The activation energies and Arrhenius prefactors obtained from the ab initio molecular dynamics simulations are used in dynamic Monte Carlo simulations to determine overall reaction rates and evolution of surface composition as a function of electrode potential.