Insights into the Mechanism of Oxygen Reduction on Platinum

Perla B. Balbuena and Daniela S. Mainardi
Department of Chemical Engineering
University of South Carolina
Columbia, SC 29208

We study the four-electron reduction of oxygen on platinum using dynamic Monte Carlo methods. Based on the comparison of two alternative mechanisms we get valuable insights into the details of the most possible pathway, including the rate determining step, the effect of ion adsorption, and adsorbate interactions. Simulated cyclic voltammetry curves such as that illustrated in Figure 1 are compared to those obtained experimentally.

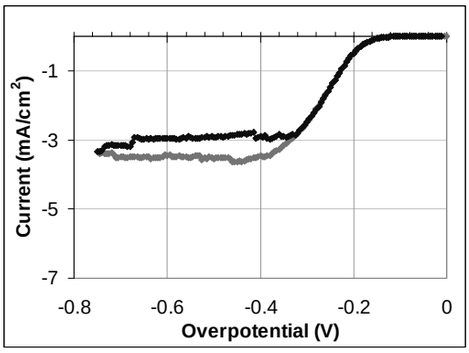

Figure 1. Simulated cyclic voltammogram for reduction of O_2 on Pt (111) where 10 % of the surface is blocked by ion adsorption.