Towards a Multiscale Model of PEM Fuel Cell Electrochemistry Using Dynamic Monte Carlo Simulations

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Slow electrochemical reactions (ECR) at the cathode of a PEM fuel cell are known to cause a substantial potential loss. These ECR are typically catalyzed by nanometer size platinum particles. The chemistry involves a number of surface species possibly involving adspecies interactions [1-2]. The inability of the mean-field approach to describe such systems accurately has been discussed widely in the literature, and dynamic Monte Carlo (DMC) simulations have been the favored choice instead [3-6].

One of the main bottlenecks in the application of the DMC method to PEM fuel cell electrochemistry has been the unavailability of rate parameters, especially for electrochemical reactions. Recent applications of *ab-initio* and DFT calculations combined with efficient optimization algorithms have led to a remarkable headway, and reasonable rata parameters are becoming increasingly available [7-8].

In this work we present DMC simulations of full PEM fuel cell electrochemistry using kinetic rate data obtained from quantum simulations. A complete sensitivity analysis of the reactions considered is also presented and the role of interactions among adsorbents is discussed. The results are compared with experimental data.

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