# Kinetic Monte Carlo simulation of the Yttria Stabilized Zirconia (YSZ) fuel cell

Kah Chun Lau

*Department of Chemistry, George Washington University, Washington D.C. 20052.*

C. Heath Turner

*Department of Chemical and Biological Engineering, University of Alabama, Bevil 132A, Box 870203, Tuscaloosa, AL 35487.*

Brett I. Dunlap

*Code 6189, Naval Research Laboratory, Washington D.C. 20375.*

A Kinetic Monte Carlo (KMC) model is developed to simulate non-symmetrically the cathode side of a Yttria Stabilized Zirconia (YSZ) fuel cell, in order to translate experimental, and ultimately theoretical rates into an atomistic model of the fuel cell [1]. The KMC model consists of a set of several electrochemical reaction rates, adopted from experiments and first-principles calculations. The KMC simulations are used to model these simultaneously occuring events, to determine potential limitations in cathode/YSZ performance. The focus of this work is ionic current density ($J$), studied as a function of various physical parameters: oxygen partial pressure ($P_{O_2}$), external applied bias voltage ($V_{ext}$), temperature ($T$), dopant concentration (mol% $Y_2O_3$), relative permittivity ($\epsilon_r$) of YSZ, and geometrical features of the YSZ electrolyte. This simple model can be used as a baseline to translate elementary chemical reaction rates into atomistic simulations of working solid oxide fuel cell cathodes, pertinent to the complete set of experimental operating conditions.

[1] K.C. Lau, C.H. Turner, and B.I. Dunlap, Solid States Ionics *(in press)*.