Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Identification of Descriptors for Oxygen Reduction Reaction on Solid Oxide Fuel Cell Cathodes DANE MORGAN, YUEH-LIN LEE, University of Wisconsin-Madison, USA, JESPER KLEIS, JAN ROSSMEISL, Technical University of Denmark, Denmark, COMPUTATIONAL MATERIALS GROUP, UW-MADISON TEAM, CENTER FOR ATOMIC-SCALE MATERIALS DESIGN, DTU TEAM — Perovskites are the major class of materials used for modern solid oxide fuel cell (SOFC) cathodes and have the ability to catalyze the oxygen reduction reaction (ORR) on their surfaces. However, difficulties in performing in-situ characterization of well-controlled samples means that the rate limiting steps and structure-property relationships underlying ORR on these materials are not understood. In particular, to date it has not been possible to find a simple set of descriptors that can be correlated to the ORR activity. A descriptor based approach has been very valuable in understanding many reactions, including the ORR, on metal catalysts (e.g. d-band center descriptor). In this talk we use an ab initio based approach to identify a descriptor for the ORR in perovskite SOFC cathodes. Energetics of key steps in the SOFC ORR are calculated for LaBO3 (B= Mn, Fe, Co, and Ni) systems and correlated with oxygen surface binding, oxygen surface vacancy formation, and oxygen band center. Reasonably good linear relationships suggest that these quantities could be effective descriptors for the ORR on SOFC perovskite cathodes.

Dane Morgan
Department of Materials Science and Engineering,
University of Wisconsin-Madison, USA

Date submitted: 09 Dec 2009 Electronic form version 1.4