**Ab initio Based Modeling of Solid Oxide Fuel Cell Cathodes**

**at the Molecular Scale**

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The performance of Solid Oxide Fuel Cells (SOFCs) depends critically on the cathode oxygen reduction reaction (ORR) activity on transition metal perovskite materials. Key challenges in understanding perovskites for SOFC cathodes include defect chemistry of bulk and surfaces/interfaces, and surface kinetics associated with the ORR. In this work we describe how *ab initio* techniques can be used to model perovskite defect chemistry in the bulk and near the surfaces/interfaces. Furthermore, a descriptor approach can be used to predict oxygen reduction catalytic activity from *ab initio* energetics and electronic structure descriptors, which opens the door to *ab initio* design of more active SOFC cathode catalysts.