**TITLE:** **Characterization of Atomic and Electronic Structures of Electrochemically Active SOFC Cathode Surfaces**

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## 1. ABSTRACT

### Objectives

The objective of this project is to understand the detailed structures of cathode surfaces in solid oxide fuel cells (SOFC) through theoretical computations coupled with *in-situ* experimental measurements. It is anticipated that the combination of theoretical and experimental approach will provide information with a level of detail that has not previously been achieved. The ultimate objective of this study is to provide some scientific basis for intelligent design of better cathode materials for SOFC based on a profound understanding of the oxygen reduction mechanism at the molecular level.

### Accomplishments to Date

Several cathode surface models have been constructed for electronic structure calculations using periodic density functional theory (DFT). In particular, DFT calculations have been used to compute the electronic structure, defect structure, and ionic conductivity of electrode materials, to identify the active reaction sites for oxygen adsorption and dissociation, to estimate the vibrational frequencies of various surface bonds/species, to construct potential energy surfaces (PESs) for various oxygen-reduction pathways, and to predict the most favorable reaction pathways or the most probable oxygen reduction mechanism.

### Future Work

Work to be performed includes probing the surfaces of selected cathode materials using *in-situ* vibrational spectroscopy to verify experimentally the vibrational frequencies predicted by DFT calculations and to identify the spectral feature associated with each cathode material that responds to perturbations under desired SOFC operating conditions.

Other tasks to be performed include to determine catalytic properties of the cathode materials using impedance spectroscopy (IS), which will be compared with the *ab initio* results by quantum-chemical calculations, and to develop scientific principles useful to intelligent design of better cathode materials for SOFCs.

## 2. LIST OF PUBLISHED JOURNAL ARTICLES, COMPLETED PRESENTATIONS, AND STUDENTS RECEIVING SUPPORT FROM THE GRANT

### Published Journal Articles

- None.

### Completed Presentations

- None.

### Students Receiving Support from the Grant

- Harry Abernathy, School of Materials Science & Engineering, Georgia Tech
- John Bennett, School of Materials Science & Engineering, Georgia Tech.