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Optimization of Oxygen Exchange Membranes through Unraveling the Contribution of Structural Rigidity via Neutron Diffraction Studies

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Progress of the Research

The goal of this project is to use neutron diffraction, on both the long-range and local length scales, to understand the role of structural rigidity in the transport of oxygen through the membrane and thus the success of different oxide structures as mixed ionic-electronic conduction membranes (MIECM). MIECM are used in as membranes to realize a cheaper route to pure oxygen extraction from air, an important reagent for the petroleum industry. To achieve this goal the project has been broken in to two different objectives.

I. Determine how diffraction derived Debye temperature can be used as a proxy for structural rigidity on the long-range and local scale using neutron diffraction techniques.
II. Elucidate other geometric parameters that could affect structural rigidity or act as a proxy for the prediction of rigidity toward the creation of design principles for MIECM materials using correlation diagrams.

The realization of objective I has several parts that cover the project duration, several of which have already been realized. A unique aspect of this research is that neutron beam time requires a proposal to be funded early on in the project. In the Fall of 2018 we were successful in obtaining beam time for the proposal *Unraveling the oxygen motion in oxygen transport membranes*. The total time requested was 4 days with an estimated value of $38,400, the full amount was obtained. This time is awarded based on a peer review of the proposed work and the funding rate less than 25%. Successfully obtaining this award required 2 students to upscale the reaction from 0.5 grams to 8 grams for 4 separate compounds and testing their stability under different conditions (Figure 1). Unfortunately, the key neutron experiment has not been performed because the Spallation Neutron Source at Oak Ridge National Laboratory (the only facility worldwide where this experiment can be done) has had several unplanned long term outages that have postponed the experiment twice. Travel arrangements were made and cancelled twice for this experiment, due to these unforeseeable outages. However, the experiment is currently scheduled for December 18-22, 2019 and two undergraduate students will be attending this experiment. Furthermore, we have already begun the synthesis and preliminary analysis of the second family of compounds that are to be analyzed via neutron diffraction so that the next beam time proposal can be submitted during the project duration. Furthermore, the large-scale samples were analyzed for magnetic and electrical properties on a recent trip to the University of Canterbury to work with a new collaborator, Dr. Donna Arnold. These are additional measurements previously unexpected, that will add to our full understanding of these material systems and thus aid in the completion of objective 1 and additional papers on these interesting systems.

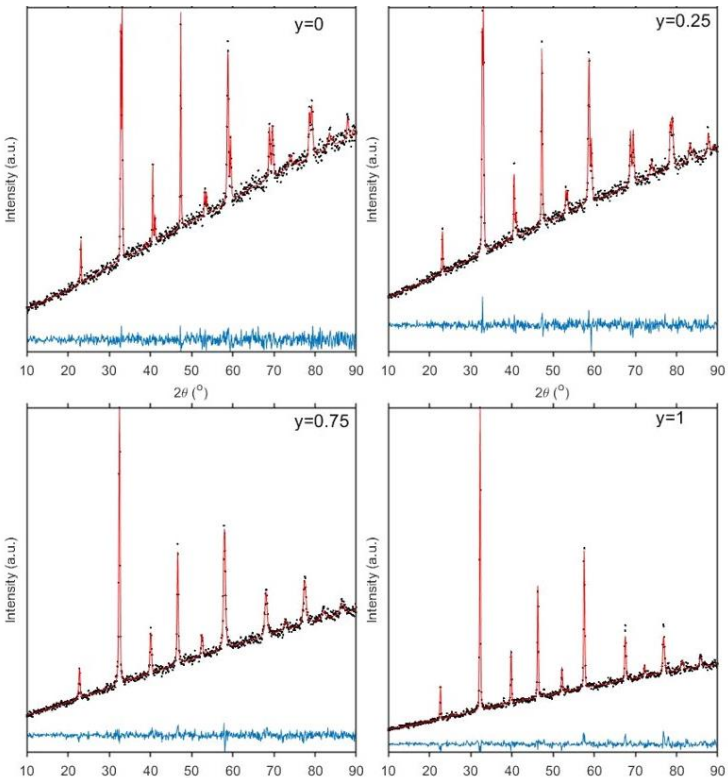

Figure 1. Laboratory powder XRD for $La_{0.9}Sr_{0.1}Co_{1-y}Fe_yO_{3-\delta}$ (y=0, 0.25, 0.75, 1). Increase in the background is due to absorption of the Cu radiation by Fe. Black dots are experimental data, red line is the calculated data via the Rietveld refinement, and the blue curve is the difference between experiential and calculated. All 4 show good agreement between the data and the model and show no indication of impurity phases.

Objective II relies on the creation of a database for machine learning and the implementation of machine learning algorithms. The creation of the database was carried out by two students over the last year and contains data for over 2000 compounds. This database not only supports this project, but is crosscutting into other projects of interest in our lab. Due to both the funding of this project by PRF and the progress made in the first 6 months of the project I was able to secure a collaboration with Dr. Sam Behseta, a statistician at CSUF specializing in machine learning. Together we have compiled a team of four undergraduates and two masters students to aid in the exploration of machine learning on this database. This aspect of the project has received further competitive funding through the California State University Chancellors office and is supported by the National Institute of Health Big Data Discovery and Diversity grant.

Impact of the research on my career and students

The funding of this project has had an impact on myself and my students over the last year. This funding has acted as seed funding that has helped me secure additional funds and collaborations as listed above. Furthermore, the beam time allotment has established me as one of the leaders in the area of exploring both solid dynamics as well as methods that allow us to probe those dynamics. This funding has also supported students getting involved in undergraduate and masters level research, which has been shown to improve both soft and technical skills. Once neutron data has been collected students will have the opportunity to present their research locally and nationally.