Faculty of Science and Engineering

2020 Australian Government Research Training Program Scholarships

Strategic Project Profile

PROJECT TITLE: Multi-metal oxide energy materials: Structural characterisation and electrochemical performance

FIELD OF RESEARCH CODE:

PROJECT SYNOPSIS:

Multi-metal oxides have been extensively investigated and utilised as electrode and electrolyte materials in energy conversion and storage areas such as advanced batteries, super capacitors, electro catalysts for water electrolysis and fuel cells. For example, perovskites (La,Sr)MnO3, (La,Sr)(Co,Fe)O3, (Ba,Sr)(Co,Fe)O3 and Layered cobaltite perovskites with general formula LnBaCo2O6-δ (Ln = Gd, Pr, Y, La, Sm and Nd) show high electro catalytic activity not only for the oxygen reduction reaction for high temperature solid oxide fuel cells, but also for the water electrolysis at room temperatures in alkaline solutions. Other technologically important materials include 3D oxide spinels, such as CuCo2O4 and NiFe2O4 and the layered oxide Ruddleson-Popper phases, such as

LnxSr4-xFe3O10-δ (Ln =La, Nd; 0 < x < 4.0).

The performance and durability of these materials are closely related to the position of various cations in different crystallographic sites and microstructures. Take a typical A-site cation ordered layered double perovskite oxide based on PrBaCo2O6-□ as an example. The balance between electrical and ionic conductivity is related to the electron hopping along the Co-O-Co bonds. The transformation of a cubic single perovskite to such a layered double structure reduces the oxygen bonding strength in the BaOδ layer and provides disorder-free channels for ion motion, which remarkably enhances oxygen diffusivity and opens the possibility for developing a new class of materials suitable for application as oxygen electrodes for solid oxide fuel cells as well as electrolysis cells.

However, the fine tuning of multi-metal oxide structures critically depends on the crystalline phase formation during the high temperature synthesis process. The high temperature sintering could come with a potential price of contamination by unwanted phases during synthesis. On the other hand, the surface segregation and subsequent reaction between the segregated species and unwanted phases could play a critical role in the interfacial reaction and subsequent the performance and stability of multi-metal oxide-based electrodes. The inter-relationship between surface segregation, reaction and interface formation are most important for the electrochemical activity of multi-metal oxide-based materials for batteries, super capacitors, and fuel cells.

This project would look at developing new multi-metal oxide materials with an emphasis on crystallographic purity and structural analysis through X-ray and neutron diffraction, pair-distribution analysis and focussed-ion beam/scanning transmission electron microscopy, as well as electrochemical analysis under fuel cell and electrolysis operating conditions. The objectives of the project are to identify the fundamental relationships between the electro-catalytic activity, microstructure, crystalline phase, and surface segregation properties under energy application conditions, such as fuel cells and electrolysis cells.

FEASIBILITY AND RESOURCING – DESCRIPTION OF THE SUPPORT THIS PROJECT WILL RECEIVE:

A wide range of multi-metal oxides will be synthesised. Electrochemical characterisation, materials synthesis, and chemicals will be made available through FETI. Materials characterisation instrumentation will be made available through the JdLC, and will include XRD/SAXS, SEM, XPS and FIB-STEM. Costs for access will come from a subscription paid from GRS funds. Access to neutron and synchrotron facilities will be by competitive proposals. Chemical costs will be paid from ARCDP project (DP180100568). Synthesis and electrochemical analysis training and support will be provided through Prof. Jiang and his research group. Structural characterisation training will be provided through Dr Rowles and the XRDSF.

WHAT MINIMAL ATTRIBUTES AND SKILLS EXPECTED BY THE CANDIDATE BE COMPETITIVE:

The candidate would require a First Class Honours, or Master's degree in physics, chemistry, or chemical engineering, or relevant experience. They would need to have an interest in energy materials, electrochemistry, and/or materials characterisation. The candidate would need effective written and oral English communication skills. Demonstrated conceptual, analytical and problem-solving skills with the ability to undertake research and analysis tasks. Skills in programming and handling large amounts of data would be desirable. Previous experience in crystallography or X-ray diffraction would he highly regarded.

THE SIGNIFICANCE OF THE PROJECT/ PROGRAM FOR THE ENROLLING SCHOOL OR INSTITUTION:

Energy is a top priority research area of the School, with the University establishing a state-of-the-art Resources and Chemistry Precinct, Institute of Functional Molecules and Interfaces, and Fuels and Energy Technology Institute, as well the facilities of the John de Laeter Centre. FETI is a primary research institute of excellence in energy and fuels, recognised locally and internationally. The proposed project will be carried out within FETI and JdLC. This project will substantially enrich our knowledge in the fundamental understanding of the relationship

between the crystalline structure, electrochemical catalytic activity, and electrode/electrolyte interfaces of multi-metal oxides as energy materials.

Students are advised to contact the Project Lead listed below prior to submission of their scholarship application to discuss their suitability to be involved in this strategic project.

PROJECT LEAD CONTACT

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PRIMARY SUPERVISOR

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