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## Insight into the Variations of ABO<sub>4</sub> Structures: Combined Experimental and Computational Studies

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The development of carbon-neutral energy-generation is critical to combatting climate change. One such technology is the development of next-generation ion conductors for solid-oxide fuel cells (SOFCs). SOFCs offer a more efficient method of extracting energy from hydrogen or hydrocarbon fuels than current combustion engines due to their one-step chemical process. However, a bottleneck to the large-scale uptake of SOFCs is the poor performance of the conducting electrolytes that separate the anode from the cathode. Various ABO<sub>4</sub> structures have recently been proposed as solid electrolyte candidates in SOFCs, with increased high-temperature ionic conductivity being measured in chemically doped LaNbO<sub>4</sub>. However, the various phase transitions of these materials within the operational temperature of SOFCs makes them non-ideal.

To understand the effects of chemical doping on the structure and electrochemical properties, several complex ABO<sub>4</sub> structures have been investigated. In this work, we present the solid-solution series  $Ln(Nb_{1-x}Ta_x)O_4$  ( $Ln = La-Lu$ ). Using a combination of synchrotron X-ray and neutron powder diffraction methods, these studies have revealed several anomalies across the series. The structures appear to be sensitive to the size of the  $Ln$  cation and their synthesis conditions, with a difference in ionic conduction performance being observed. This experimental data has been further reinforced by ground state energy calculations performed using density functional theory. This is a landmark accomplishment that has not been previously used in similarly studied structures. These insights can be used in the development and engineering of novel and advanced electrolyte materials for SOFCs.

### Level of Expertise

Student

### Presenter Gender

Man

### Pronouns

He/Him

### Which facility did you use for your research

Australian Centre for Neutron Scattering

### Students Only - Are you interested in AINSE student funding

Yes

### Do you wish to take part in the Student Poster Slam

## Condition of submission

Yes

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