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Insight into the Variations of ABO_4 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_4 structures have recently been proposed as solid electrolyte candidates in SOFCs, with increased high-temperature ionic conductivity being measured in chemically doped $LaNbO_4$. 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_4 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.

Presenter Gender

Man

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

Students Only - Are you interested in AINSE student funding

Yes

Level of Expertise

Student

Pronouns

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Which facility did you use for your research

Australian Centre for Neutron Scattering

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