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Examination of the local and average structure of disordered perovskites for ionic conduction

Dr Frederick Marlton, *Chancellor's Research Fellow at the University of Technology Sydney (UTS).*

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Time: 1:00 – 2:00PM
Venue: Room 107, Woodside
20 Exhibition Walk, Monash Clayton Campus

Abstract

The flexible structure of perovskites enables the incorporation of anion vacancies, making them attractive materials for ion conduction applications. Calcium titanate-based compounds exhibit oxygen ionic and electronic conductivity, and have the potential to be used in high-temperature electrochemical devices due to their moderate thermal expansion and stability in reducing atmospheres. The ionic conductivity can be altered by partially replacing the Ti^{4+} cations with lower valent cations, such as Fe^{3+}. The perovskite system $CaTiO_3$ – $CaFeO_{2.5}$ exhibits an increase in oxygen vacancies, from zero in $CaTiO_3$ to 0.5 per formula unit in $CaFeO_{2.5}$ (or $Ca_2Fe_2O_5$), which adopts the brownmillerite structure. Several studies have been conducted on the $CaTi_{1-x}Fe_xO_{3-x/2}$ system using a combination of Mössbauer spectroscopy, microscopy and diffraction techniques. An early study revealed that with increasing Fe content, the anion vacancies go from completely disordered at low Fe contents, to a fully ordered from. This evolution from a disordered to ordered arrangement of vacancies is important as it affects the structure of the system and, in turn, the ionic conductivity. In this work we used a combination of high-resolution X-ray diffraction, X-ray Spectroscopy and neutron total scattering to understand the local and average structure of $CaTi_{1-x}Fe_xO_{3-x/2}$ for $x \leq 0.4$. This revealed significant disordering of the oxygen framework, which has implications for tuning the ionic conductivity.

Biography

Dr Frederick Marlton is a Chancellor's Research Fellow at the University of Technology Sydney (UTS). After completing his Science and Engineering degrees from the Australian National University, Fred moved to Sydney to complete a PhD at the University of New South Wales. His project was supervised by John Daniels and focused on combinatorial methods for synthesising lead-free piezoelectrics. Fred then conducted postdocs at Aarhus University with Mads Jorgensen (MAX IV) and at the University of Sydney with Chris Ling and Brendan Kennedy. After a brief stint in consulting, optimising train networks for iron-ore mining, Fred started his fellowship at UTS in 2023.

The focus of Fred's research is structure property relationships in functional metal-oxide materials. Specifically, Fred specialises in understanding the local structure via neutron and X-ray pair distribution function (PDF) analysis. This has been applied to a variety of interesting materials, such as perovskite ferroelectrics, scheelite photocatalysts and pyrochlore ionic conductors. Recently, Fred was awarded a Fulbright to conduct a 6-month research project with the Karunadasa group at Stanford University, investigating the local structure of novel halide perovskites for semiconductor applications.

Convener: Professor Laure Bourgeois
Email: mcem@monash.edu Tel: 9905 5563

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