Oral presentation

# Structural Investigations of a Family of Perovskite-Derived Oxide Ion Conductors

**Oliver J Wagstaff[1], Ivana R Evans[1] and John S O Evans[1]**

[1] *Department of Chemistry, Durham University, Durham, DH1 3LE, United Kingdom*

oliver.wagstaff@durham.ac.uk

The global transition away from dependence on fossil fuels necessitates the development of devices that can utilise alternative fuel sources such as hydrogen. Solid oxide fuel cells (SOFCs) are one technology that benefits from high energy conversion efficiencies and a lack of moving parts. Traditional materials used to form the oxide ion conducting electrolyte in SOFCs (e.g., yttria-stabilised zirconia, YSZ or gadolinia-doped ceria, GDC) suffer from poor intercomponent compatibility and require high temperatures (>1000 °C) to conduct sufficiently for use in fabricated devices, which reduces cell lifetimes. This presents an opportunity for the discovery of novel materials that produce better quality devices.

Whereas the mechanisms of ionic conductivity in YSZ and GDC have been well understood through their simple defect chemistry, more recently investigated materials use more complex mechanisms of ionic conductivity. These mechanisms involve features such as flexible coordination spheres (e.g., $La_2Mo_2O_9$ (LAMOX) materials) and terminal oxygen sites unconnected to the wider polyhedral framework (e.g., $La_{1.54}Sr_{0.46}Ga_3O_{7.27}$ (melilite)), which both help stabilise migrating oxide ions through local relaxation, affording greater ionic conductivity [1,2].

The $A_3OhTd_2O_{7.5}$ materials (A = alkaline earth, Oh = octahedral, Td = tetrahedral metal ions) are a family of oxygen-deficient perovskite derivatives identified as structurally interesting potential ionic conductors because they adopt a variety of structures with chains containing $Td_2O_7$ moieties (figure 1a) [3,4]. These groups possess two terminal oxygens per unit and (for materials with Td = Ga) variable coordinate metal centres. There has also been evidence of order-disorder phase transitions involving the oxygen substructure, further suggesting high ionic mobility and conductivity [5].

We will present results of combined X-ray and neutron diffraction studies on members of the $A_3OhTd_2O_{7.5}$ family including $Ba_{1.5}Sr_{1.5}YGa_{2-x}Zn_xO_{7.5-\delta}$ and $Ba_3ScGa_2O_{7.5}$. The former are mixed A-site materials formed by the intergrowth of Ba/Sr-rich regions and exhibit additional oxygen substructure disorder within the $Ga_2O_7$ units. $Ba_3ScGa_2O_{7.5}$ has been shown to have a previously uncharacterised orthorhombic structure formed by supercell ordering of a simple distorted perovskite cell. The supercell was identified through additional electron diffraction measurements.

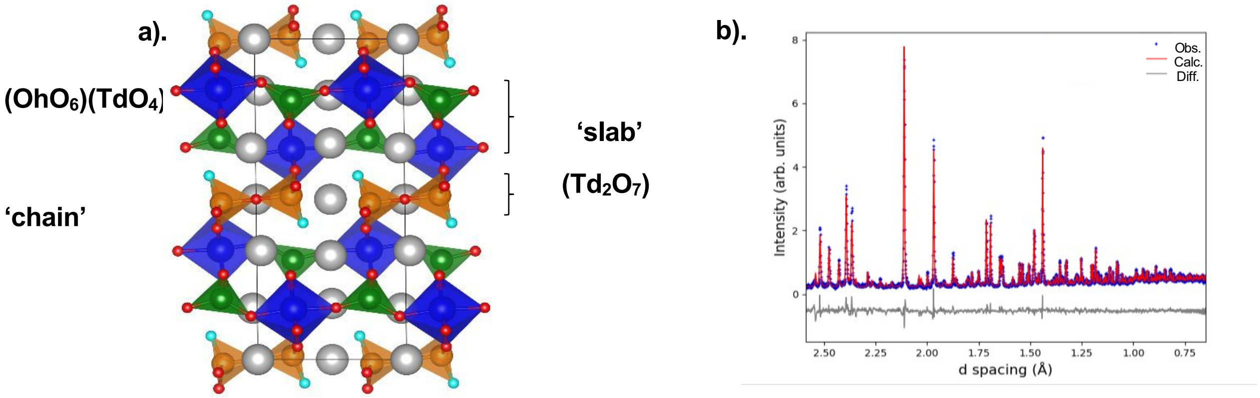

**Figure 1** – a). Example of an $A_3OhTd_2O_{7.5}$ structure (A - grey, Oh - blue, Td - green/orange, O - red. Terminal O-sites are highlighted in light blue). b). Rietveld refinement against room temperature neutron data for $Ba_{1.5}Sr_{1.5}YGa_2O_{7.5}$.

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