

Oral Contributions

[MS28 - 03] **Oxide Ion Conductors for Energy Applications: Twists and Hops in the Solid State.** Ivana Radosavljević Evans^{1,*}, Xiaojun Kuang¹, Julia L. Payne¹, James D. Farrell¹ and Mark R. Johnson²

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Meeting the future energy needs of the world's growing population is one of today's most significant scientific challenges. Different types of new, renewable and sustainable energy generation have been the subject of intense research, including solar, nuclear, wind and geothermal energy. Solid oxide fuel cell (SOFC) technology is a frontrunner in the short-to-medium term race to provide sustainable energy solutions, owing to the unique combination of high efficiency, fuel flexibility and environmental safety. Two factors have prevented the widespread commercialisation of SOFCs: system cost and reliability, and both stem from the high operating temperatures of the current technology (850–1000°C). Lowering the operating temperatures into the so-called intermediate temperature region (500–700°C) is therefore a major driver in SOFC research. An in-depth understanding of the structural features associated with high ionic mobility is essential for the successful discovery and preparation of new oxide ion conductors capable of overcoming the limitations of the currently used materials. As materials structural complexity increases, crystallographic characterisation using a range of techniques (powder and single crystal, X-ray and neutron, *in-situ* studies) and state-of-the-art diffraction data analysis approaches, aided by DFT molecular dynamics simulations, is essential in providing this insight. We have recently reported exceptional low-temperature oxide ion conductivity in

$\text{Bi}_{1-x}\text{V}_x\text{O}_{1.5+x}$ ($x = 0.095\text{--}0.087$) phases, with $\sigma = 3.5\text{--}10^{-2}$ S/cm at 450°C, the highest to-date in a stable

3D fluorite-type system. We have attributed this remarkable behaviour to the simultaneous presence of four key structural factors: a highly polarisable sublattice with vacancies, central atoms able to support variable coordination numbers and geometries, and the rotational flexibility of these coordination polyhedra, co-existing in a pseudo-cubic structure.[1] We have found similar structural features to lead to high oxide ion conductivity in a number of other materials with complex superstructures (vanadates, molybdates, tungstates, rhenates). [2-5] This presentation will focus on the new materials discovered and characterised and the crystallographic methods used to characterise them.

In particular, it will emphasise how a combination of careful crystallographic work, computational methods and characterisation of physical properties is required to understand the complexity of next-generation functional materials. The methods adopted are relevant and widely applicable to energy-related and other functional materials.

[1] X.J. Kuang, J.L. Payne, M.R. Johnson, I.R. Evans, *Angewandte Chemie International Edition* **51** (2012) 690.

[2] X.J. Kuang, Y.D. Li, C.D. Ling, R.L. Withers, I.R. Evans, *Chemistry of Materials* **22** (2010) (15) 4484.

[3] X.J. Kuang, J.L. Payne, J.D. Farrell, M.R. Johnson, I.R. Evans, *Chemistry of Materials* **24** (2012) (11) 2162.

[4] C.D. Ling, W. Miiler, M.R. Johnson, D. Richard, S. Rols, J. Madge, I.R. Evans, *Chemistry of Materials* **24** (2012) (23) 4607.

[5] J.L. Payne, M.R. Johnson, I.R. Evans, *Unpublished results* (2013).