[5] Ch. Baerlocher, F. Gramm, L. Massueger, L. B. McCusker, Z. B. He, S. Hovmöller, X. D. Zou, *Science* **2007**, *315*, 1113-1116.
[6] Ch. Baerlocher, D. Xie, L. B. McCusker, S. J. Hwang, I. Y. Chan, K. Ong, A. W. Burton, S. I. Zones, *Nature Mater*. **2008**, *7*, 631-635.
[7] D. Xie, Ch. Baerlocher, L. B. McCusker, *J. Appl. Cryst.* **2011,** *44*, 1023-1032.
[8] A. W. Burton. US Patent 7820141, 2010.
[9] D. Xie, L. B. McCusker, Ch. Baerlocher, *J. Am. Chem. Soc.* **2011,** *133*, 20604-20610.

Keywords: powder diffraction; structure solution; charge flipping

MS46-O2 **Neutron Scattering Studies of Ionically Conducting Oxides.** Stephen Hull [a], Stefan T. Norberg [ab], Sten G. Eriksson[b]. [a]*The ISIS Facility, Rutherford Appleton Laboratory, Didcot, Oxfordshire, OX11 0QX, United Kingdom,* [b]*Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-41296 Gothenburg, Sweden.*
E-mail: stephen.hull@stfc.ac.uk

Solid Oxide Fuel Cells (SOFCs) are an important technology in the quest for more environmentally benign power generation. A key component within an SOFC is the solid electrolyte, which transfers O^{2-} ions from the air side (cathode) to the fuel side (anode) of the cell, with a compensating flow of electrons in the opposite direction through an external circuit which provides the electrical power. As a consequence, the material chosen for the role of the solid electrolyte must possess a high oxide-ion conductivity and low electronic conductivity (the latter essential to avoid internal short-circuits). At present, the most widely used material for the solid electrolyte in SOFCs is yttria stabilised zirconia (YSZ, $Zr_{1-x}Y_xO_{2-x/2}$ with x typically around 0.15). However, these SOFCs must be operated at temperatures of ~1200K to achieve a sufficiently high ionic conductivity within the YSZ electrolyte. There are a number of advantages of SOFC operation at lower temperatures (~600-900K), including reduced problems of corrosion and shorter start-up times, which have motivated considerable research effort to identify materials with higher values of ionic conductivity than YSZ. These include the related material $Zr_{1-x}Sc_xO_{2-x/2}$ and solid solutions based on Bi_2O_3 and CeO_2, which all possess an anion-deficient fluorite crystal structure (space group).

This presentation will briefly summarise our recent programme of neutron powder diffraction studies of the SOFC materials mentioned above, performed at the ISIS spallation neutron source. Particular emphasis will be devoted to the following aspects.

(*i*) The use of 'total scattering' methods (*i.e*. considering bith the Bragg and diffuse scattering components), including reverse Monte Carlo analysis of the data to probe the nature of the defects within the materials.

(*ii*) The complimentary use of neutron powder diffraction and Molecular Dynamics simulations to investigate the nature of the ionic diffusion mechanisms and the factors which promote extensive oxide-ion diffusion.

(*iii*) The development of novel sample environment devices to allow neutron powder diffraction studies of SOFC electrolyte materials to be performed under conditions of temperature and gas atmosphere which mimic those found in real device applications.

Keywords: solid oxide fuel cells; neutron powder diffraction; reverse Monte Carlo