

“On the design and development of ion conducting oxides”

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There are major initiatives around the world with a focus on enabling the “Hydrogen Economy”, with the hope that this can become part of a clean, sustainable alternative to fossil fuels. One key aspect of that is the development of proton conducting materials for fuel cells and hydrogen separation membranes. To better understand the design of improved proton conducting ceramics, we have undertaken a study that combines synthesis, neutron scattering and computational investigations. Highly conducting fluorite and perovskite related ceramics have been characterized using quasielastic scattering, powder diffraction, and vibrational spectroscopy at the Spallation Neutron Source. Here we present recent work looking at the use of this combined computational/experimental approach to understand the mechanism of proton conduction, and consider implications on the design of new materials.