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Structural features of a new oxygen deficient perovskite oxygen ion conductor explored by neutron scattering

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Oxygen ion conductors are materials of major interest for a series of application in the area of solid state ionics. In particular, oxides with brownmillerite type structure (A2BB'O5) have attracted much attention, showing oxygen ion mobility down to ambient temperature.

Brownmillerite type frameworks containing B-cations with saturated or empty electron shells (d0 or d10 configurations) present a special case, as they impose a fixed oxygen stoichiometry, making them good candidates to study oxygen diffusion mechanisms on a microscopic level. In this context, we have synthesized a new phase (Sr2ScGaO5), having pure oxygen ion conductivity. Depending on the synthesis route, it adopts two polymorphs: the orthorhombic brownmillerite, consisting of alternating octahedral and tetrahedral layers, or an oxygen deficient cubic perovskite structure. Once synthesized, both phases are surprisingly kinetically stable, rendering them as a model system to study oxygen diffusion mechanisms.

We report here on a multi-technical approach to characterize structural changes as a function of temperature. High-resolution structure analysis has been performed using X-rays (synchrotron and laboratory) and neutron diffraction methods, combined with neutron PDF analysis for local environment. To better understand the oxygen mobility mechanisms, these studies were complemented by Raman and impedance spectroscopy.

Corallini S. et al, J. Phys. Chem. C 2015, 119, 11447-58. Ceretti M. et al, Crystals 2016, 6 (11), 146. Corallini S. et al. Inorg. Chem. 2017, 56, 2977-84. Ceretti M. et al., Inorg. Chem. 2020, 59, 13, 9434-42

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