

MaMaSELF

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Pr₂NiO_{4+δ} structure, valence states and lattice dynamics investigated by synchrotron radiation.

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Oxides, exhibiting high oxygen ion conductivity, have gained considerable interest for their applications in Solid Oxide Fuel Cells (SOFCs). However, still today high operation temperatures of about 1000 °C are needed for SOFCs, requiring huge problems of mechanical and chemical stability. Unfortunately, a decrease in the temperature reduces activity of the solid electrolyte and reactivity of the cathode. Thus, a better understanding of the diffusion process on a microscopic scale is fundamental in optimizing SOFCs.

Perovskite type oxides, ABO₃, and their derivatives, such as layered Ruddlesden-Popper nickelates, (LnO)(LnNiO₃)_n, where Ln is an alkaline earth or rare earth metal, show interesting ionic and electronic transport properties. In addition, oxygen mobility related to low-energy phonon modes has been observed in SrFeO_{2.5}, which gives evidence of a phonon-assisted diffusion mechanism in solids.

To investigate the high oxygen mobility present in Pr₂NiO_{4+δ}, at already moderate temperatures, structure, valence states and lattice dynamics are investigated in the present master thesis project. In situ single crystal X-ray diffraction will be carried out in a special electrochemical cell to change stoichiometry in a controlled way. This will allow to correlate a crystal structure as a function of δ . XES will be carried out in situ in order to investigate changes in the electronic structure upon reduction of Pr₂NiO_{4+δ}. Inelastic X-ray scattering will be used to correlate the existence of low-energy phonon modes with the oxygen stoichiometry. The synthesis of polycrystalline electrodes and single crystals are carried out at the University of Montpellier, all characterizations given above will be performed at the ESRF.

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