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Synthesis, structure, valence state and physical properties in Fe-containing perovskite matrix for energy materials

Due to the demands on energy, the search and improvement of energy materials have become one of the most popular topics around the world. Among them, the development of oxygen ion conductor is receiving increasing attention due to its importance in solid oxide fuel cells (SOFCs), batteries, electrodes, sensors, and catalysis. SOFCs, for example, has several advantages over other types of fuel cells, including high power generation efficiency and high impurities resistance in the fuel. However, the operation of SOFC requires high temperature, which often leads to compound degradation and indirectly limits the choice of acceptable materials [1].

In this regard, brownmillerite type structure has been reported as a promising candidate material showing oxygen mobility at ambient temperature. A system such as Sr2ScGaO5 has been fully investigated through structural analysis, lattice dynamics etc[2]., in order to understand the fundamentals of oxygen mobility mechanism.

Inspired by the previous work, this project aims to replace Ga with Fe and explores the effect of iron valence state which no one has reported. Our major interest is driven by the ability of iron to adopt various oxidation states Fe2+(FeII), Fe3+(FeIII), Fe4+(FeIV), with fixed, closed-shell Sc3+substitution. The doping concentration remains constant as x = 0.5 in SrScxFe1-xO3- δ (SFSO); while the oxygen non-stoichiometry is between $2.5 \le 3-\delta \le 2.75$ by topotactic redox process. The valence state is expected to compensate for oxygen and changes the structure, electrical properties as well as magnetic properties. Preliminary analysis by X-ray diffraction (XRD), Thermogravimetry Analysis (TGA) with Mass Spectroscopy (MS), and Superconducting Quantum Interference Device (SQUID) is performed at the Institut Charles Gerhardt Montpellier (ICGM). Oxygen content and local structure are obtained by high-resolution two-axis neutron powder diffractometer (D2B) at the Institut Laue Langevin (ILL, Grenoble, France). High-resolution X-ray spectroscopy at the ESRF is also performed to obtain the local electronic structure because of its sensitivity of iron valence states.

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