

# Oxygen defects in Sr<sub>2</sub>FeO<sub>4</sub>: a computational study

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Sr<sub>2</sub>FeO<sub>4</sub> (SFO) is the first-order Ruddlesden-Popper (RP) perovskite-type material, a prospective positron material for solid oxide and proton-conducting electrochemical cells. In materials of this type oxygen defects (vacancies and interstitials) strongly affect proton conductivity. The main goal of the present study is a detailed description of processes of oxygen defects' formation and migration in SFO. All results of this study are obtained by means of the DFT+U method.

We have calculated oxygen vacancy (Vo) formation energies in non-stoichiometric Sr<sub>2</sub>FeO<sub>4-δ</sub> for δ=0.125, 0.25, 0.5. The spatial distribution of vacancies has been varied to identify and calculate all symmetrically inequivalent configurations. Preferred oxygen vacancy migration pathways have been traced. Vo migration energy was calculated for δ=0.125. Spatial distribution of vacancy-induced polarons has been mapped. We conclude that Vo migration occurs predominantly within the perovskite layer of the RP structure.

The second type of oxygen defect, oxygen interstitial (Oi) has been modelled in a form of anti-Frenkel pair. Two primary types of Oi in the SFO structure have been identified: an off-site single oxygen and an off-site oxygen bonded with a lattice oxygen, forming a dumbbell configuration. The latter, when connected to both Sr and Fe, was found to be the most favourable interstitial configuration. From the calculated values of Oi migration energies we conclude that migration of Oi is energetically preferable within the SrO layer of the RP structure. The present investigation on oxygen defects in Sr<sub>2</sub>FeO<sub>4</sub> is a solid foundation for the further proton transport studies.

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