**Molecular Dynamics Studies of Structure and Oxide Ion Transport in Sr doped LaFeO3**

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**Abstract**

Classical molecular dynamics simulations have been employed to investigate the structure and oxide ion transport in Sr doped LaFeO3 [La1-XSrXFeO3-δ] for a wide range of composition (x=0.1-0.6) to gain insights into the process. The lattice parameter of the material shows very small variation with increasing Sr concentration, while the self-diffusivity of the oxide ions as well as the resulting ionic conductivity decreases. It is observed that the oxygen migration occurs through the edges of the octahedra and only of intra-octahedra type, agreeing well with previously reported study.

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