

Elektrocheminēs Medžiagotyras Seminaras

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First principles calculations of protonic defects in ferrate perovskites

Among ceramic fuel cells, protonic ceramic fuel cells (PCFC) attract a growing interest. Proton-conducting ceramic electrolytes offer higher ionic conductivities compared to oxide ion conductors, in particular at intermediate temperatures ($T = 300\text{-}600^\circ\text{C}$). Finding optimum cathode materials with mixed protonic and electronic conductivity is crucial for the PCFC performance. Protons are incorporated by either hydration (filling of oxygen vacancies), or hydrogen uptake from H_2O by a redox reaction. So far, proton concentrations were measured only for a few cathode materials, e.g. $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Fe}_{0.8}\text{Zn}_{0.2}\text{O}_{3-\delta}$ perovskite. They are significantly smaller than for $\text{BaZr}_{1-x}\text{Y}_x\text{O}_{3-x/2}$ electrolyte materials under comparable conditions. An atomistic understanding of the parameters determining proton uptake is, therefore, of great importance.

In the present study, we perform first principles calculations for nonstoichiometric $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$ and $\text{Ba}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$ as potential PCFC cathode materials, with and without protons. These simulations yield detailed information on various possible point defect configurations. This makes it possible to look for correlations of their formation energies with other properties such as ion charges, local coordination, bond lengths etc. This allows us to obtain an atomistic understanding of the key parameters determining proton uptake in PCFC cathode materials.

