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Oxygen vacancy equilibrium concentrations in strontium-doped lanthanum cobalt iron oxides HENG LUO, XI LIN, Boston University — Formation of oxygen vacancies by introducing various mixed-valent cation dopants is a common procedure to improve the cathode performance in solid oxide fuel cells. A generic computational procedure is developed in this work to predict the oxygen vacancy equilibrium concentrations at experimentally relevant temperatures and oxygen partial pressures for both bulk and surface oxide phases. The calculations are based on the first-principles density functional theory and a constrained free-energy functional. Quantitative agreements are found by direct comparisons to the thermogravimetry measurements for various strontium-doped lanthanum cobalt iron oxides. Our results indicate that the oxygen vacancies are energetically stabilized at surfaces for all temperatures and all oxygen partial pressures, while such surface stabilization effects become stronger at higher temperatures and lower oxygen partial pressures.

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