Effects of Zn Doping on Proton Conduction in Ba(Co0.4Fe0.4Zr0.1Y0.1)O3-δ Perovskite: Distance and Directionality

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Abstract

Ion doping is generally an effective strategy for improving the electrochemical performance of electrode materials in protonic ceramic fuel cells (PCFCs). However, the specific mechanism by which the dopant affects proton transfer remains unclear. Inspired by the excellent proton uptake ability of BaCo0.4Fe0.4Zr0.1Y0.1O3-δ, a transition-metal-doped perovskite oxide, we investigate the influence of Zn doping on the proton transport characteristics using first-principles methods. The dopant is revealed to enhance proton conductivity through both distance and directionality effects. Zn substitution at the Zr site facilitates the formation of oxygen defects, and this effect is particularly strong for the first-nearest neighbor oxygen atoms. In addition, interactions between the dopant and adjacent oxygen atoms increase the negative charge density (i.e., alkalinity) of the nearest bonding oxygen atoms, which is conducive to proton uptake. Moreover, the dopant promotes proton migration along adjacent oxygen atoms, with directionality from O34 (Y–O34–Zn) to O23 (Zn–O23–Zr). Our findings demonstrate that Zn-doped BaCo0.4Fe0.4Zr0.05Zn0.05Y0.1O3-δ is a promising oxide material with triple conductivity. This analysis provides a general strategy for efficient doping to optimize proton conductivity in perovskite oxides.

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