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Investigation of the Effect of Yttrium Doping on Oxygen Ion Diffusion in Zirconia using DFT Method for Enhancing SOFC Electrolyte Design

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Abstract
Solid Oxide Fuel Cells (SOFCs) have gained significant attention as a developing technology for clean and sustainable energy production. The electrolyte, a key component of SOFCs, is crucial in optimizing their performance. Enhancing oxygen ion conductivity in these electrolytes is essential for improving the efficiency and reducing the operating temperature of SOFCs. One effective approach is doping the electrolyte with impurity elements. Thus, the main objective of this research is to investigate the influence of yttrium doping on oxygen ion diffusion in zirconia, the most commonly used commercial electrolyte. Using Density Functional Theory (DFT) calculations, the effect of yttrium doping and its position on the activation energy was examined. The results indicate that yttrium, regardless of its doping position in zirconia, reduces the activation energy for oxygen ion diffusion. However, the position of the yttrium significantly affects the diffusion pathway, as oxygen prefers to diffuse through a path where the yttrium is absent. Furthermore, the results suggest that yttrium creates preferred oxygen vacancy sites within the structure.

Keywords: solid oxide fuel cell, solid electrolyte, density functional theory, ionic diffusion, atomic doping,

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