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Theoretical and experimental study of $Ca_xCe_{1-x}O_{2-\delta}$ electrolyte for SOFCs

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Calcium doped ceria ($Ca_xCe_{1-x}O_{2-\delta}$,x = 0.03, 0.12, 0.19) electrolyte was synthesized using co-precipitation method for low temperature solid oxide fuel cell. The composition CDC3 ($Ca_{0.19}Ce_{0.81}O_{1.90}$) shows the highest ionic conductivity of 0.095 Scm-1and lowest activation energy of 0.49eV. First-principle calculations based on density functional theory are performed to investigate the doping effects of Ca in ceria $Ce_{0.81}Ca_{0.19}O_{1.90}$ (CDC3). The influence of first, second and third oxygen vacancy in Ca-doped ceria is investigated theoretically. It is observed that oxygen vacancies tend to increase the lattice parameter and decrease the bulk modulus. Dopant-vacancy association energies and vacancy formation energies are calculated to reveal the doping effects on oxygen ion conduction. The effect of first, second and third oxygen vacancy on the density of states and band gap was discussed. This analysis gives a useful idea of vacancy diffusion that could be beneficial in optimizing doping materials for enhancing oxygen ion conductivity in doped ceria.

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