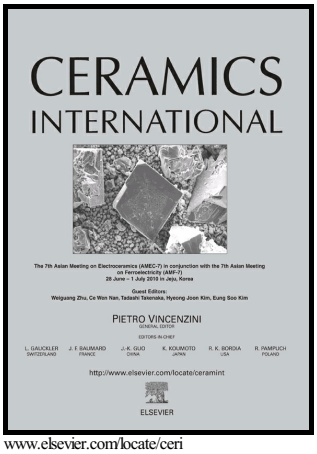

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A potential electrolyte ($Ce_{1-x}Ca_xO_{2-\delta}$) for fuel cells: Theoretical and experimental study

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Abstract

First-principles calculations are performed using density function theory to explore the effects of dopant Ca in ceria ($Ce_{1-x}Ca_xO_{2-\delta}$). The impact of oxygen vacancy on band gap and density of states is examined in doped ceria using generalized gradient approximations. Vacancy association and vacancy formation energies of the doped ceria are calculated to reveal the effect of dopant on ion conduction. The experimental study of the sample ($Ce_{0.875}Ca_{0.125}O_{2-\delta)}$ was performed to compare with the theoretical results. The obtained results from theoretical calculation and experimental techniques show that oxygen vacancy increases the volume, lattice constant (5.47315 Å) but decrease the band gap (1.72 eV) and bulk modulus. The dopant radius (1.173 Å) and lattice constant (5.4718 Å) are also calculated by equations which is close to the DFT lattice parameter. The result shows that oxygen vacancy shifts the density of states to lower energy region. Band gap is decreased due to shifting of valence states to conduction band. Vacancy formation shows a significance increase in density of states near the Fermi level. Density of states at Fermi level is proportional to the conductivity, so an increase in density of