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Effect of Fe doping on O vacancy/interstitial formation and migration in PrBaCo₂O_{5+d} OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — Oxygen vacancy formation and migration are key factors considered for the operation of cathodes in solid oxide fuel cell. First-principles calculations are used to investigate Fe doped PrBaCo₂O_{5+d} as cathode material for intermediate temperature solid oxide fuel cells. We discuss the electronic properties of the pristine system and the effect of Fe doping on the structural and electronic properties. Different concentrations of the dopants are calculated. We find that the volume of the unit cell and O vacancy formation energy increase linearly with the Fe content concentration. We also investigate the formation of oxygen interstitial as a function of Fe substitution and the possibility of anisotropic diffusion of the O ion was also studied.

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