

## Influence of CA, SR and BA Substitution on lafeo3Performances During Chemical Looping Processes

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**Abstract :** La-based perovskite oxygen carriers, especially the doped-La(M)FeO<sub>3</sub>, showed excellent performances during chemical looping processes. However, the mechanisms of the undoped and doped La(M)FeO<sub>3</sub> are not clear at present, making the mechanisms clear may help the development of chemical looping technologies. In this paper, the method based on the density function theory (DFT) was used to analysis the influence of Ca, Sr, and Ba doping of La on the electronic structure, while the CO oxidation mechanisms on the surface of LaFeO<sub>3</sub> and Ca-doped LaFeO<sub>3</sub> oxygen carriers were also analyzed. The results showed that the band gap was decreased by the doping of low valence. While the doping of low valence element Ca, Sr, and Ba at La site simultaneously resulted to the moving of the valence band toward high energy and made the valence band cross the Fermi energy level. This was resulted from the holes generated by divalent ion substitution. The holes can change the total magnetization from antiferromagnet to weakly ferromagnetism. The calculation results about the formation of oxygen vacancy showed that substitutions of Ca, Sr, and Ba caused a large drop in oxygen vacancy formation energy, indicating that the bulk oxygen transport was improved. Based on the optimized bulk of the undoped and Ca-doped LaFeO<sub>3</sub>(010) surface, the CO adsorption was analyzed. The results indicated that the adsorption energy increased by divalent ion substitution, meaning that the adsorption stability decreased. The results can provide a certain theoretical basis for the development of perovskite oxides in chemical looping technologies.

**Keywords :** chemical looping technologies, lanthanum ferrate (LaFeO<sub>3</sub>), divalent ion substitution, CO oxidation

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