

## First-principles calculations of thermodynamic driving force for cation segregation on perovskite-type materials

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Cation segregation leads to various product phases at the surfaces and interfaces of solid oxide fuel cell (SOFC) cathodes. It has the direct relations to control the oxygen reduction reaction and stability of SOFC cathode. Therefore, identifying the thermodynamic driving force for cation segregation plays an important role in designing high performance SOFC cathodes.

In this study, we investigated the thermodynamic behavior of cation segregation in two classes of perovskite-type materials using density DFT calculations. The first class is alkaline earth metal (Ba, Sr, and Ca)-doped  $\text{LaBO}_3$  ( $B = \text{Cr}_{0.50}\text{Mn}_{0.50}, \text{Mn}, \text{Fe}, \text{Co}_{0.25}\text{Fe}_{0.75}, \text{Co},$  and  $\text{Ni}$ ) perovskites and the second class is  $\text{SrTi}_{1-x}\text{Fe}_x\text{O}_3$  ( $x = 0.00, 0.25, 0.50, 0.75, 1.00$ ) perovskites. While the dopant segregation (Ba, Sr, and Ca) is observed in the first class, lattice cation (Sr) segregation is observed in the second class. Although there are two different mechanisms in cation segregation, the mainly driving force is similar for both cases. We found that the strain effect induced size difference of A-site and B-site cations in perovskite oxides is the most dominant driving force.