Mechanistic Study for Metallic Nano Particle Exsolution on $PaBaMn_{2-x}M'_xO_{5+\delta}$ (M' = Co and Fe) Perovskite

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Double layered $PrBaMn_2O_{5+\delta}$(PBMO) is known as a noble anode material for solid oxide fuel cells (SOFCs) due to its facile redox stability with higher tolerance of coking or sulphur poisoning from hydrocarbon fuels. Recently, several experimental results showed that the metallic Co can be exsolved from PBMO under reducing atmosphere. When the Co is doped into a host perovskite lattice during the synthesis in the reducing atmosphere, some of the metals can be exsolved from bulk toward the surface. After the exsolution, well-distributed active metallic nanoparticles are formed. In this study, we reveal the mechanism of Co or Fe exsolution on double layered $PaBrMn_2O_{5+\delta}$, demonstrating that oxygen vacancy formation and segregation energy can be used as descriptive factors to quantitatively analyze the possibility of exsolution. On the basis of these results, we briefly introduce our results for the screening of exsolution preferences for several precious metals on a wide range of $ABB'O_3$ perovskite oxides using DFT calculations. Our computational screening procedure will be useful to explore the promising perovskite supporting materials.