Mechanistic Study for the Formation of Exsolved Alloy Nanoparticles on Transition Metal Doped $PaBaMnO_{5+\delta}$ under Reducing Environment

김경학, 한정우†
포항공과대학교
(jwhan@postech.ac.kr†)

The exsolution phenomena of B-metal dopants on perovskite oxide supports have been received a lot of attention due to the formation of well-distributed active metallic nanoparticles (NPs) under reducing atmosphere. Separately, it has been known that the cell performance of $PrBaMn_2O_{5+\delta}$ (L-PBMO) is significantly enhanced with the Co-Fe alloy catalyst when C_3H_8 and CH4 are used as a fuel into the anode of solid oxide fuel cells. Recently, the formation of exsolved alloy NPs on L-PBMO was also reported, which can be a useful strategy to synthesize the oxide-supported alloy NPs. However, the detailed mechanism for such phenomena on L-PBMO is not unclear. In this study, we suggest two possible mechanisms of "Bulk alloy formation" and "Surface alloy formation" to unveil the mechanism of the exsolution of Co-Ni alloy NPs on L-PBMO. Our DFT calculations demonstrated that the exsolution of Co-Ni alloy NPs is thermodynamically favorable through "surface alloy formation mechanism".