

B-metal exsolution on layered perovskite: From potential driving forces to catalytic activity

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B-metal exsolution has great potential to synthesize well-distributed metal nanoparticles (NPs) on the surface of oxide support materials. In previous works, we found the different exsolution tendencies of different kinds of transition metals on double-layered PrBaMn<sub>2</sub>O<sub>5+δ</sub> (L-PBMO). In particular, the exsolved NPs showed higher catalytic activity and stability for fuel oxidation, such as dry reforming of methane. Based on our density functional theory (DFT) results, we will introduce (1) a possible driving force for B-metal NPs exsolution, (2) thermodynamically favorable mechanism for alloy NPs exsolution, (3) catalytic activity of exsolved NPs, and (4) how to boost B-metal exsolution to further improve cell performance SOFCs with the experimental verifications.