Theoretical study on exsolution catalyst for high-temperature water gas shift reaction

임채성, 한정우†, 양희재, 황루이
POSTECH
(jwhan@postech.ac.kr†)

High-temperature water gas shift (HT-WGS) reaction is one of the main gas reforming reactions for hydrogen production. The conventional HT-WGS catalysts have stability issue due to the sintering of nanoparticles (NPs) at high temperature. Recently, exsolution catalyst (Ni NP at $LaFeO_3$ perovskite) was developed as a highly stable HT-WGS catalyst. For the rational design of the improved exsolution catalyst at the atomic scale, the theoretical study is required.

In this study, we performed theoretical study on exsolution catalyst for HR-WGS using density functional theory. We designed NP model as exsolution catalysts which have exsolved metal, support, and interfacial sites. To determine the validity of theoretical model, we compared theoretically calculated activation energy with experimentally measured one (Ni NP at $LaFeO_3$ perovskite). Then, we used [Co-Fe alloy NP at $(PrSr)_{0.5}Fe_{1-x}Co_xO_3$ perovskite] as a model exsolution catalyst to reveal the role of B-metal doping and oxygen vacancy on HT-WGS. These results may guide the development of improved exsolution catalyst for HT-WGS reaction.