

Investigating mechanism of reverse water–gas shift reaction on CeO₂–based catalyst by density functional theory

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Global warming has been accelerated due to the increase in emission of greenhouse gas, CO₂, causing serious problems in environments and climates. Thus, the regulation on CO₂ emission has been reinforced and utilization of CO₂ has been studied. However, CO₂ molecule is chemically and thermodynamically stable. Therefore, activation and conversion of CO₂ to valuable products is attracting worldwide attention. Reverse water–gas shift (RWGS) reaction is one of the promising processes that utilizes CO₂ to produce syngas, since the syngas can be converted into valuable carbon–based chemicals by Fischer–Tropsch process. CeO₂–based catalysts showed high performance in RWGS due to its oxygen mobility and re–oxidation of oxygen vacancy by CO₂. Moreover, strong metal–support interaction (SMSI) between CeO₂ and active metals induces high reducibility of CeO₂ and high dispersion of metals. In this study, we tried to investigate the mechanism of RWGS on CeO₂–based catalysts using density functional theory (DFT) calculation.