Mechanistic Insight into the Conversion of CH_4 and CO_2 to Acetic Acid on CeO_2-ZnO

고정현, 한정우†
서울시립대학교
(jwhan@uos.ac.kr†)

The synthesis of acetic acid has received wide attention because of the industrial applications. At present, the most widely used method for acetic acid production depends on the indirect multiple step processes. However, it requires harsh reaction condition and different types of catalysts in each step. On the contrary, direct conversion of CH_4 and CO_2 into acetic acid can take place under mild temperature and atomic economic reaction. One of the main challenges is that this direct conversion is thermodynamically unfavorable. Thus, it is required to introduce a novel concept to overcome the thermodynamic limitation. In this study, we employed a CeO_2-ZnO/MMT catalyst, which provides dual active sites, and also is known to show a higher catalytic activity. To understand a role of each active site, we examined the successive steps of the co-conversion of CH_4 and CO_2 into acetic acid on CeO_2(111) and O-terminated ZnO(0001) via density functional theory (DFT) calculations. Through the DFT analysis of different steps on each surface with experimental evidence, we elucidated the reaction mechanism of co-conversion of CH_4 and CO_2 to acetic acid on CeO_2-ZnO/MMT. Our results will provide mechanical insight the reason why CeO_2-ZnO/MMT catalyst exhibits better catalytic activity.