Reaction mechanism of Dimethyl ether Carbonylation to Methyl acetate over Ferrierite Zeolite : a First-principles Study

김효석, 박명준[1], 이원보†
서울대학교; [1]아주대학교
(wblee@snu.ac.kr†)

Dimethyl ether (DME) has been a promise source to produce olefin or hydrocarbon because of its environmental sustainability and economic feasibility. One of main reaction of the DME conversion is the DME carbonylation reaction to methyl acetate (MA), which is catalyzed by Zeolites. However, the detail reaction mechanism is still unclear because of its complexity of atomic structure. In the presentation, a reaction mechanism on Ferrierite zeolite is suggested and the energy pathway is calculated using First-principles calculation. The rate determining step is verified using transition state theory and the role of Bronsted acid site and the origin of high selectivity are also discussed in the presentation.