

Importance of Zn in Enhancing the Activity and Stability of the Kinked Cu(211) Surface in CH<sub>3</sub>OH Production by CO<sub>2</sub> Hydrogenation and Dissociation : First-principles Microkinetic Modeling Study

조덕연, 함형철<sup>1</sup>, 이관영<sup>†</sup>

고려대학교 화공생명공학과; <sup>1</sup>한국과학기술연구원

(kylee@korea.ac.kr<sup>†</sup>)

Cu based catalysts have been used variously to synthesize valuable potential hydrogen source like a methanol and formic acid from CO<sub>2</sub> therefore recent studies have been targeting raising effectiveness of catalysts. In this study, to find actual effect of Zn in Cu alloy, we modeled four surfaces such as terrace, step, defected step and alloy. We found that favorable site separations are occurred in Zn with oxygen included intermediates and carbon based intermediates. Moreover, we found the most probable energetics pathways in CO<sub>2</sub> to MeOH reaction with a DFT study over all of facets and it was observed that an activation barrier in HCOO route was the lowest in Zn.