Microkinetic Modeling for Methanol Synthesis on Cu through CO_2 and CO Hydrogenation and Water-Gas-Shift Reaction: A Combined DFT and UBI-QEP Method Considering Coverage Effects

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C1 chemistry is a technology that produces a variety of useful chemicals from one carbon material such as CH_4, CO and CO_2. This study deals with the process of producing methanol on copper from syngas ($CO/CO_2/H_2$) and, firstly, focus on reaction energetics of the mechanism. Then microkinetic modeling is conducted through 28 elementary steps. These steps include CO_2 and CO hydrogenation and water-gas-shift reaction. Kinetic parameters are estimated with a combination of density functional theory (DFT), the semi-empirical unity bond index-quadratic exponential potential (UBI-QEP) method, and transition-state theory (TST). Using DFT, the preferred adsorption site, adsorption energy, and gas phase enthalpy of each species are obtained. The activation energy is obtained from UBI-QEP and the pre-exponential factor from TST. Also, by combining DFT and UBI-QEP, the adsorption energy and activation energy can be obtained considering coverage effects. With the microkinetic model, kinetic information such as the most abundant surface species, rate-limiting steps, and methanol production rates is obtained.