Structural Sensitivity of Hydrogenation in Carbon Dioxide to Methanol Synthesis over Cu by means of coordination numbers : A DFT Study

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Methanol has been used as a base chemical and has also been suggested as a stable transportation fuel in carbon industry. Methanol synthesis path was developed in 1923 years and Cu/ZnO/Al2O3 catalyst has been used commonly so copper is still known for carbon hydrogenation-favor metal. Recently, synthesis method of nanoparticle catalysts has been developed so a role of their structural sensitivity or defected facet effect would be a important issue as an activity variable. We present density functional theory (DFT) calculations for CO2 hydrogenation by calculating chemisorption energies of intermediates on three different Cu facet surfaces: face centered cubic (111) terrace, (211) step and (211) kink. Our DFT calculations show that CO2* -> CO*+O* reaction, the energetics was most preferred as 0.468 eV on (211) kink but 2.210 eV on (211) step and then CO*+H* -> HCO* hydrogenation reaction, it was estimated over 1.897 eV on both kink and step but 0.836 eV on terrace. Such a different energetics would affect each hydrogenation path or reduction so facet effect would have important role in determining overall reaction path.