pH effects on the electrochemical reduction of CO(2) towards C2 products on stepped copper - DTU Orbit (30/01/2019)

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We present a microkinetic model for CO(2) reduction (CO(2)R) on Cu(211) towards C2 products, based on energetics estimated from an explicit solvent model. We show that the differences in both Tafel slopes and pH dependence for C1 vs C2 activity arise from differences in their multi-step mechanisms. We find the depletion in C2 products observed at high overpotential and high pH to arise from the 2nd order dependence of C-C coupling on CO coverage, which decreases due to competition from the C1 pathway. We further demonstrate that CO2 reduction at a fixed pH yield similar activities, due to the facile kinetics for CO2 reduction to CO on Cu, which suggests C2 products to be favored for CO2R under alkaline conditions. The mechanistic insights of this work elucidate how reaction conditions can lead to significant enhancements in selectivity and activity towards higher value C2 products.

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