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Theoretical Investigation on the Electroreduction of CO_{2} to Methanol on Stepped Cu-based Alloy (211) Surfaces

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A systematic investigation of CO_{2} electroreduction to CH_{3}OH on copper-based alloys stepped (211) surfaces was performed using density functional theory calculations associated with the standard hydrogen electrode model. The interaction of the key C_{x}H_{y}O_{z} intermediates is shown to be related to the CO adsorption energy due to the similar charge transfer characteristics of the C–O bond in CO*and those intermediates. The overpotential, the limiting-potential elementary step, and selectivity to CH_{4}, CH_{3}OH, and HCOOH are determined. The competitive reaction of H_{2} evolution is also investigated. The results demonstrate that the CO* protonation is the limiting-potential step on most surfaces, with the exception on Cu_{3}Au and Cu_{3}Co surfaces. Methanol production is favorable on Cu_{3}Pd and Cu_{3}Pt surfaces, yet they show high overpotential (~0.7 V). In spite of the excessive strong CO*interaction on some surfaces, the overpotential may be reduced on the surface which is able to decouple the CO* adsorption energy and HCO*/COH* adsorption energy. The key of methanol selectivity is CH_{2}OH*intermediate formation favorability associated with the preference of CH_{2}OH* protonation at the C atom over the O atom. The calculations reveal that the electroreduction activity on Cu-based alloys catalysts do not show a volcano-type relation as was previously found on pure metal catalysts.

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