Electrochemical CO_2 reduction to formate via oxygen bidentate intermediate on high-index planes of dendritic Bi catalyst

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Conversion of CO_2 and water to value-added chemicals powered by renewable electricity is a promising strategy for sustainable industrial development. For the success of this approach, in-depth understanding of catalysis on CO_2 converion is firstly required because it involves highly complex multistep reactions. Herein, we report a rational design of a hierarchical Bi dendrite catalyst for an efficient CO_2 to formate production. A high reactivity and a stable performance during long-term operation were achieved with the Bi dendrite (~89% at −0.74 V_{RHE} during 12 h). Density functional theory (DFT) is used to investigate three possible reaction pathways in terms of surface intermediate, and the one via *OCOH surface intermediate is calculated to be the most energetically feasible. DFT calculations further elucidate the plane-dependent catalytic activity and conclude that the high-index planes developed on the Bi dendrite are responsible for the outstanding performance of Bi dendrite. We expect that our experimental and theoretical study will provide a fundamental guideline for the CO_2-to-formate conversion pathway as well as design principles for enhancing the catalytic performance.