Systematic Screening Study for Metal-Nitrogen-Doped Carbon Catalysts in CO_2 Electrochemical Reduction

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Electrochemical CO_2 reduction reaction (CO_2RR) is a promising approach to close the CO_2 cycle. Metal nitrogen-doped carbon (M-N-C) catalysts have been focused as favorable catalysts for CO_2RR towards CO production. For an efficient design of M-N-C catalyst, it is necessary to establish a systematic theory-derived screening process combined with the experimental validation. In this study, using DFT calculations, we first screened the M-N-C through the active site poisoning and the formation energy. To define the descriptor for CO_2RR activity and selectivity, the free energy diagrams of CO_2RR and HER were derived. The screened M-N-C was experimentally synthesized using a metal-organic framework (MOF) to measure CO_2RR activity and selectivity. In all potential ranges, the maximum reaction energy could be considered a key descriptor describing the CO partial current density. On the other hand, the Faradaic efficiency could be explained as the difference of the *CO and *H binding energy in the low potential region (-0.6 V_{RHE}) and *CO desorption in the high potential region (-1.1 V_{RHE}).