Effective Screening Route for Highly Active and Selective Metal-Nitrogen-Doped Carbon Catalysts in CO_2 Electrochemical Reduction

박병준, Ying Wang, 이예찬, 한정우†
포항공과대학교
(jwhan@postech.ac.kr†)

Electrochemical CO_2 reduction reaction (CO_2RR) is a promising approach to close the CO_2 cycle as waste CO_2 into a useful chemical. We present a screening route that uses density functional theory calculations to figure out high-efficiency metal−nitrogen−doped (M–N–C) catalysts for the CO_2RR. Twenty-three M–N–C catalysts were evaluated, and three M–N–C (M = Fe, Co, or Ni) were identified as promising candidates and tested as proof-of-concept catalysts. We propose different key descriptors, including the maximum reaction energy, differences of the *H and *CO binding energy ($\Delta G_{*H} - \Delta G_{*CO}$), and *CO desorption energy ($\Delta G_{*CO \rightarrow CO(g)}$) to clarify the reaction mechanism at different potential region. These computational descriptors effectively predicted the experimental observations in the entire range of electrochemical potential. This screening route provides a guideline for the rational design of heterogeneous CO_2RR electrocatalysts.