Rational engineering local structures of single-atom catalysts for selective CO_2 electroreduction

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CO_2 electrochemical reduction reaction (CO_2RR) has attracted significant attention for converting CO_2 into value-added feedstock under ambient conditions as the concentration of atmospheric CO_2 continue to increase. Recently, nitrogen doped carbon-based materials including transition metals (M-N-C) have emerged as promising alternatives for CO_2RR.

Herein, we synthesized metal nitrogen-doped carbon catalysts (M-N-C, M = Fe, Co, and Ni) using ZIF-8 as a metal-organic framework. The transition metals (Fe, Co, and Ni) were selected by a systematic computational screening study of 23 kinds of M-N-C catalysts based on activity, selectivity, and stability. As for Fe-N-C catalyst, the FE_{CO} reached a maximum of 90 % at low overpotential region. Co-N-C and Ni-N-C catalysts obtained their maximum FE_{CO} of 50 % and 80 % respectively at intermediate overpotential region. Interestingly, when Fe-N-C and Ni-N-C were annealed under mixed gas atmosphere (H_2 and Ar), FE_{CO} further increased to 97 % and 98 % respectively.