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ABSTRACT:

Ni single Atom Decorated Catalysts for Electrochemical CO_2 Conversion

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The pursuit of a circular carbon economy and the need to surmount the constraints of electrocatalytic CO2 reduction reaction (CO2RR) technology have prompted the development of single-atom catalysts (SACs) for electrocatalysts. SACs need supporting materials. Among the diverse support materials, the zeolitic imidazolate framework (ZIF) has been widely used to prepare metal-nitrogen-doped carbon (M-N-C) SACs with dense active sites. We utilized an eco-friendly approach to produce two-dimensional ZIF-8 nanosheets (ZIF-8-NS) as an optimal support material for SACs. Additionally, we introduced Ni precursor into the synthesis process of Ni-ZIF-8-NS, which was then subjected to pyrolysis at 950 °C under a N2 atmosphere to yield the final product, Ni-NC-NS. Ni-NC-NS demonstrated an outstanding CO2RR performance by exhibiting excellent Faradaic efficiency toward CO of ~100%. Developing M-N-C SACs with high loadings for the electrochemical CO2RR remains challenging owing to the risk of metal aggregation. We present a facile strategy for synthesizing M-N-C SACs using metal-chelating ligands, eliminating the need for additional processing steps. Specifically, using ethylenediaminetetraacetic acid as a strong metal-chelating ligand, we effectively prevent the formation of Ni nanoparticles and achieve a high loading of approximately 2.7 wt%, leading to the development of high-loading Ni SACs. The resulting catalysts exhibit a high CO Faradaic efficiency of 96.6% and CO partial current density of –120.2 mA cm–2 and retain a Faradaic efficiency over 90% in a broad potential range of –0.4 to –0.9 V vs. the reversible hydrogen electrode (RHE). Theoretical calculations indicate that the asymmetric Ni–N3C1 local coordination structure within the catalyst reveals an optimal balance between *COOH formation and *CO desorption, which enhances the activity for CO2RR to CO. Dual-atom catalysts (DACs) offer a potential to accelerate reaction kinetics and provide versatile active sites by the synergistic combination of two metal atoms. So, we report DACs composed of Cu/Ni species anchored on N-doped carbon (Cu/Ni-NC) for the CO2RR. Our findings reveal that a Cu–Ni atomic distance of ~4.08 Å maximizes synergistic interactions between the two metals, significantly

enhancing catalytic activity and CO selectivity. The resulting catalysts demonstrate a CO faradaic efficiency of ~100% at −0.9 V vs. the RHE in an H-type cell and 96.3% at −0.4 V vs. RHE in the flow cell, outperforming other Cu/Ni configurations and single-metal counterparts.

Keywords: carbon dioxide reduction, ZIF-8, electrocatalyst, carbon monoxide, sp2 C, local effect