Manganese single-atom catalyst boosts performance of electrochemical carbon dioxide reduction

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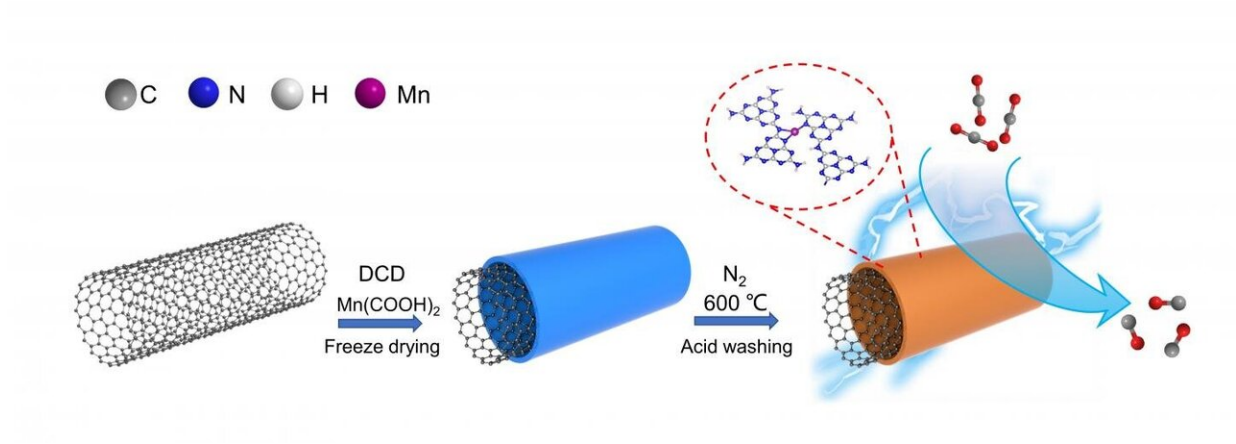

Schematic diagram of Mn SAC preparation and mechanism of electrochemical CO_2 reduction. Credit: FENG jiaqi

Electrochemical CO_2 reduction reaction (CO_2RR) is a promising approach to convert CO_2 into useful chemicals.

A research team led by Prof. Zhang Suojiang from the Institute of Process Engineering (IPE) of the Chinese Academy of Sciences prepared a manganese (Mn) single-atom catalyst (SAC) with Mn-N_3 site supported by graphitic C_3N_4, which exhibited efficient performance of CO_2 electroreduction.

This work was published in *Nature Communications* on August 28.

It is a great challenge to obtain high Faradaic efficiency (FE) and high current density simultaneously by cheap catalysts for CO_2RR.

The prepared catalyst exhibited a maximum CO FE of 98.8% with 14.0 mA cm^{-2} CO current density (j_{CO}) at overpotential of 0.44 V in $KHCO_3$ electrolyte, outperforming all reported Mn SACs.

Moreover, a higher j_{CO} value of 29.7 mA cm^{-2} was obtained at overpotential of 0.62 V, when ionic liquid was used as electrolyte.

X-ray absorption spectroscopy and high-angle annular dark-field scanning transmission electron microscopy confirmed atomically dispersed Mn in the catalyst, and the best-fitting analysis indicated that the isolated Mn atom was three-fold coordinated by N atoms.

"In situ X-ray absorption spectra and density functional theory calculations demonstrated that the remarkable performance of the catalyst was attributed to the $Mn\text{-}N_3$ site, which facilitated the formation of the key intermediate COOH through a lowered free energy barrier," said Prof. Zhang Suojiang.

This work shows that the CO_2RR activity of Mn-based catalysts can be enhanced through changing coordinated environment.

"It provides an important scientific basis and feasibility for low cost and high efficient electrochemical CO_2 reduction to useful chemicals," said Prof. Zhang Xiangping, a co-corresponding author of the paper.

More information: Jiaqi Feng et al, A Mn-N3 single-atom catalyst embedded in graphitic carbon nitride for efficient CO_2 electroreduction, *Nature Communications* (2020). DOI: 10.1038/s41467-020-18143-y

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