

Cu interface matters during CO2 electroreduction

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Graphical abstract. Credit: DOI: 10.1021/jacs.1c09508

It is attractive to convert CO_2 into multicarbon hydrocarbons and oxygenates (C_{2+} products), but it is challenging to enhance the kinetics of carbon-carbon (C-C) coupling during CO_2 reduction reaction (CO_2RR).

Cu has a superior catalytic performance in C-C coupling. However, its selectivity is undermined in a neutral medium due to the acceleration of the competing hydrogen evolution reaction (HER).

In a recent study published in Journal of the American Chemical Society,



a team led by Prof. Gao Minrui from the University of Science and Technology of China (USTC) of the Chinese Academy of Sciences developed an oxide-derived (OD)-Cu catalyst with sufficient Cu(100)/Cu(111) interfaces which displayed high Faradaic efficiency (FE) at a <u>current density</u> of 300 mA·cm⁻², and confirmed that the interfaces played a critical role in C-C coupling.

The researchers synthesized a series of OD-Cu catalysts with different facets followed by a performance test in a flow-cell with a neutral medium. They discovered that OD-Cu-III, which was composed of both Cu(100) and Cu(111) facets and had the longest Cu(100)/Cu(111) interface, exhibited superior CO₂RR catalytic performance. Meanwhile, there was a linear relationship between C₂₊ selectivity and the length of Cu(100)/Cu(111) interface, which implied that the interface might be the <u>active site</u> for C-C coupling.

The following characterizations offered a more profound explanation for the superior catalytic performance of Cu(100)/Cu(111) interface. Kelvin probe force microscopy (KPFM) revealed that the interface had the lowest contact potential difference (CPD), which was indicative of faster electron transfer and enhanced CO₂RR kinetics. Operando Raman spectroscopy, on the other hand, detected more surface-adsorbed CO (*CO) on step sites. Since step sites better contribute to the conversion of *CO to C₂₊ products, the result explained the catalysts' superior *CO dimerization ability.

Finally, density functional theory (DFT) calculations were conducted to further understand the reaction mechanism. The result showed the lowest dimerization barrier at Cu(100)/Cu(111) interface. It implied a modified electronic structure along the interface. As a result, OD-Cu-III exhibited the best CO_2RR performance.

This work determined that the Cu(100)/Cu(111) interface played a



crucial role in CO_2RR catalysis. It is of great significance for the utilization of CO_2 to prepare multicarbon fuels.

More information: Zhi-Zheng Wu et al, Identification of Cu(100)/Cu(111) Interfaces as Superior Active Sites for CO Dimerization During CO₂ Electroreduction, *Journal of the American Chemical Society* (2021). DOI: 10.1021/jacs.1c09508

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