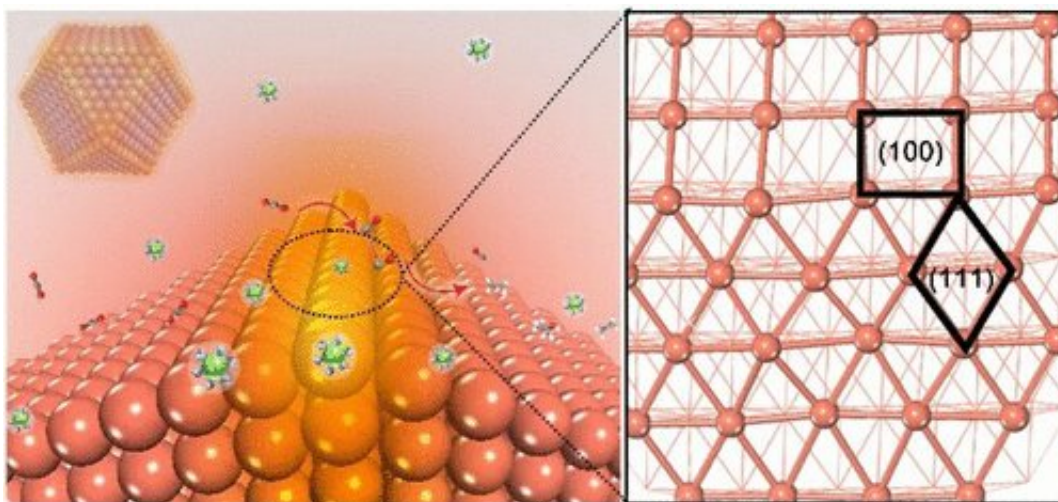


Cu interface matters during CO₂ electroreduction

January 24 2022, by Liu Jia



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

It is attractive to convert CO₂ into multicarbon hydrocarbons and oxygenates (C₂₊ products), but it is challenging to enhance the kinetics of carbon-carbon (C-C) coupling during CO₂ reduction reaction (CO₂RR).

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 [current density](#) of $300 \text{ mA}\cdot\text{cm}^{-2}$, 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 [active site](#) 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 CO₂RR performance.

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

crucial role in CO₂RR catalysis. It is of great significance for the utilization of CO₂ 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](https://doi.org/10.1021/jacs.1c09508)

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