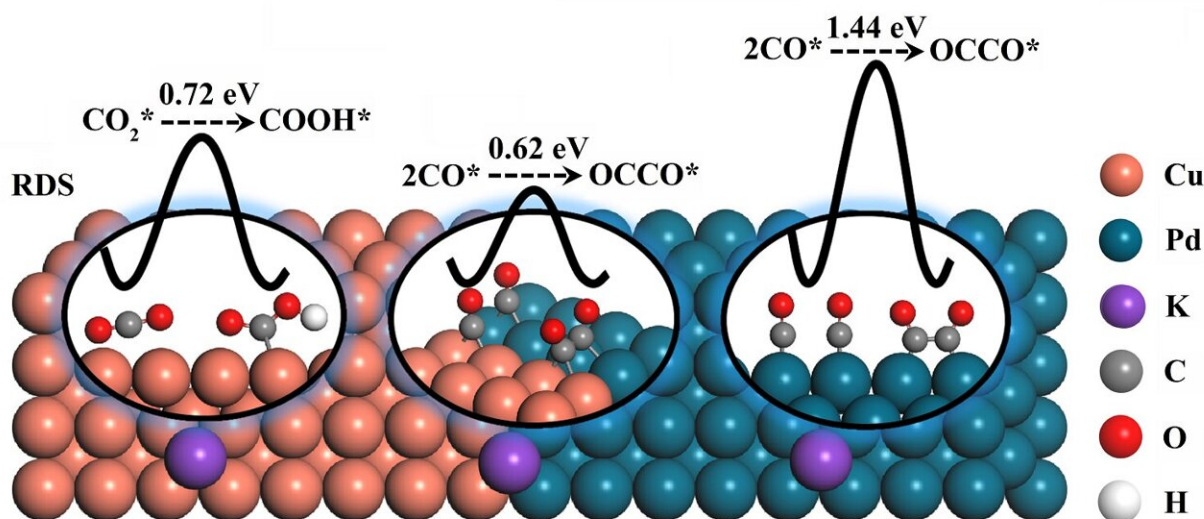


Tuning reaction barriers for carbon dioxide electroreduction to multicarbon products

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An intimate CuPd(100) interface was designed to lower the energy barriers of intermediate reaction (CO_2^* hydrogenation and C-C coupling) and improve the efficiency of C₂ products. The optimal CuPd(100) interface catalyst exhibited a C₂ Faradaic efficiency of 50.3%, which was 2.1 times higher than that of Cu catalyst (23.6%) at ~ 1.4 VRHE in 0.1 M KHCO_3 . Credit: Chinese Journal of Catalysis

Using intermittent electric energy to convert excessive CO_2 into C₂ products, such as ethylene and ethanol, is an effective strategy to mitigate the greenhouse effect. Copper (Cu) is the only single metal catalyst which can electrochemically convert CO_2 into C₂ products,

albeit with undesirable selectivity of the C₂ product. Therefore, improving the conversion efficiency of Cu-based catalysts for reducing CO₂ to C₂ products has attracted great attention.

Recently, a research team led by Prof. Min Liu from Central South University, China, designed a Cu-Pd bimetallic electrocatalyst with a CuPd(100) [interface](#) that can lower the energy barrier of C₂ product generation. The electrocatalyst was obtained via an in-situ growth method based on thermal reduction to afford Pd nanoparticles as nucleated seeds. The results were published in [Chinese Journal of Catalysis](#).

Generally, there are two limiting factors for achieving the electroreduction of CO₂ to C₂ products, namely the amount of CO* intermediate (* indicates the intermediate is adsorbed on the surface of the catalyst) and the C-C coupling step (generally two CO* coupling). For Cu catalysts, the energy barrier of the C-C coupling step is relatively low. However, the CO₂ adsorption and CO₂* hydrogenation ability of Cu are unfavorable, resulting in an insufficient amount of CO* involved in the subsequent C-C coupling step. Palladium (Pd) is an efficient catalyst that exhibited strong CO₂ adsorption and ultrafast reaction kinetics for CO* formation. However, CO* poisoning on the Pd surface makes it unsuitable for generating C₂ products. To take full advantage of both Cu (low energy barrier of C-C coupling) and Pd (ultrafast kinetics for CO* formation), the assembly of a CuPd bimetallic catalyst was envisaged as a potential method for optimizing the efficiency of C₂ product formation.

The density functional theory (DFT) calculation shows that the CuPd (100) interface enhanced the adsorption of CO₂ and reduced the energy barrier of CO₂* hydrogenation step; thus, sufficient CO* participated in the C-C coupling reaction. In addition, the energy barrier of rate-determining step for C₂ product generation on CuPd (100) interface is

0.61 eV, which is lower than that on Cu(100) surface (0.72 eV).

Then the target CuPd (100) interface catalyst was prepared by a simple wet chemical method and proved by different characterization methods. The temperature programmed desorption and gas sensor experiment results proved the enhanced CO₂ adsorption and CO₂* hydrogenation ability on CuPd(100) interface, respectively. As a result, the CuPd(100) interface catalyst exhibited a C2 Faradaic efficiency of 50.3%, which was 2.1 times higher than that of Cu [catalyst](#) (23.6%) at -1.4 V_{RHE} in 0.1 M KHCO₃. This work provides a reference for the rational design of Cu-based electrocatalyst for CO₂ electroreduction by adjusting the intermediate reaction [energy barrier](#).

More information: Li Zhu et al, Tuning the intermediate reaction barriers by a CuPd catalyst to improve the selectivity of CO₂ electroreduction to C₂ products, *Chinese Journal of Catalysis* (2021). DOI: [10.1016/S1872-2067\(20\)63754-8](https://doi.org/10.1016/S1872-2067(20)63754-8)

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