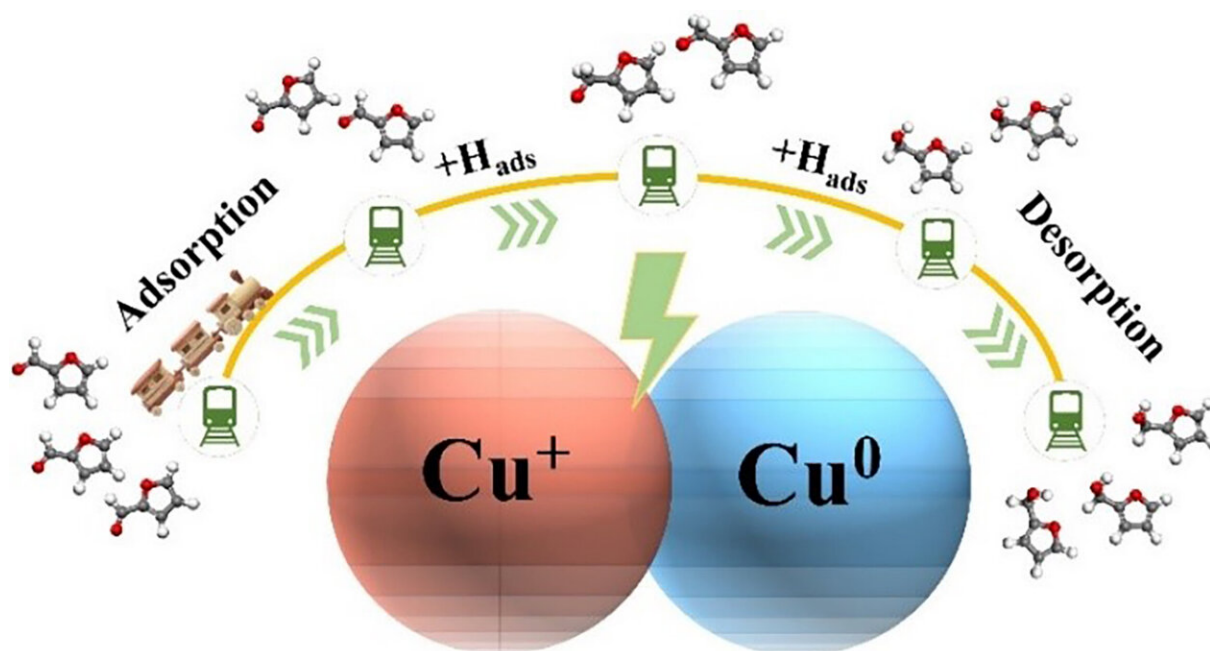


# Promoting the electrochemical hydrogenation of furfural by synergistic $\text{Cu}^0$ - $\text{Cu}^+$ active sites

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The  $\text{Cu}^0$ - $\text{Cu}^+$  synergistic effect is beneficial to both kinetics and thermodynamics:  $\text{Cu}^+$  accelerates the second-step hydrogenation process of furfural, and  $\text{Cu}^0$  reduces the energy barrier for the desorption of furfuryl alcohol. Credit: Science China Press

In a study published in *Science China Chemistry* and led by Prof. Yuqin Zou (College of Chemistry and Chemical Engineering, Hunan University), experiments were performed by using a series of in situ

characterization and the density functional theory (DFT) calculation.

It is noteworthy that the experimental findings show that  $\text{Cu}^0$  catalyzed furfural hydrogenation without  $\text{Cu}^+$  possesses a slow hydrogenation rate and poor selectivity. In contrast, the  $\text{Cu}^0$ - $\text{Cu}^+$  [active sites](#) possess excellent performance in the selective hydrogenation of furfural to produce furfuryl alcohol.

Moreover, this catalytic advantage shows a clear potential dependence, with a regular decrease in furfural selective hydrogenation performance when a decrease in potential leads to a decrease in the proportion of  $\text{Cu}^+$ .

"Cu-based catalysts have shown excellent catalytic performance for the electrochemical hydrogenation of furfural to produce furfuryl alcohol. However, the true reaction [active site](#) remains unclear. Mixed-valence Cu oxide catalysts demonstrate excellent furfuryl alcohol selectivity but are limited by the dynamic electrocatalyst surface during catalysis. In situ capture of the true reaction activity sites and thus insight into the origin of the Cu-based catalyst furfural electrochemical hydrogenation activity is necessary. This work could inform the optimal design of all Cu based catalyst electrocatalytic hydrogenation processes for organics," Zou says.

Herein, the oxidation state of the prepared CuO nanowire under the ECH of furfural was tracked by in situ X-ray absorption spectroscopy (XAS). The co-existence of  $\text{Cu}^0$  and  $\text{Cu}^+$  states during the electrohydrogenation was confirmed. Moreover, the poisoning experiment proved the decisive role of  $\text{Cu}^+$  in the furfural ECH.

Finally, the reaction energy barriers of the furfural ECH on  $\text{Cu}(111)$ ,  $\text{Cu}_2\text{O}(111)$ , and  $\text{Cu}^0$ - $\text{Cu}^+$  were analyzed by the density functional theory (DFT) calculation. It is concluded that  $\text{Cu}^0$ - $\text{Cu}^+$  active sites on the surface of CuO synergistically the conversion of furfural to furfuryl

alcohol, and the respective roles of  $\text{Cu}^0$  and  $\text{Cu}^+$  have also been revealed:  $\text{Cu}^+$  accelerates the second-step [hydrogenation](#) process of furfural, and  $\text{Cu}^0$  reduces the [energy barrier](#) for desorption of furfuryl [alcohol](#).

**More information:** Zhongcheng Xia et al, Promoting the electrochemical hydrogenation of furfural by synergistic  $\text{Cu}^0$ - $\text{Cu}^+$  active sites, *Science China Chemistry* (2022). [DOI: 10.1007/s11426-022-1407-0](https://doi.org/10.1007/s11426-022-1407-0)

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