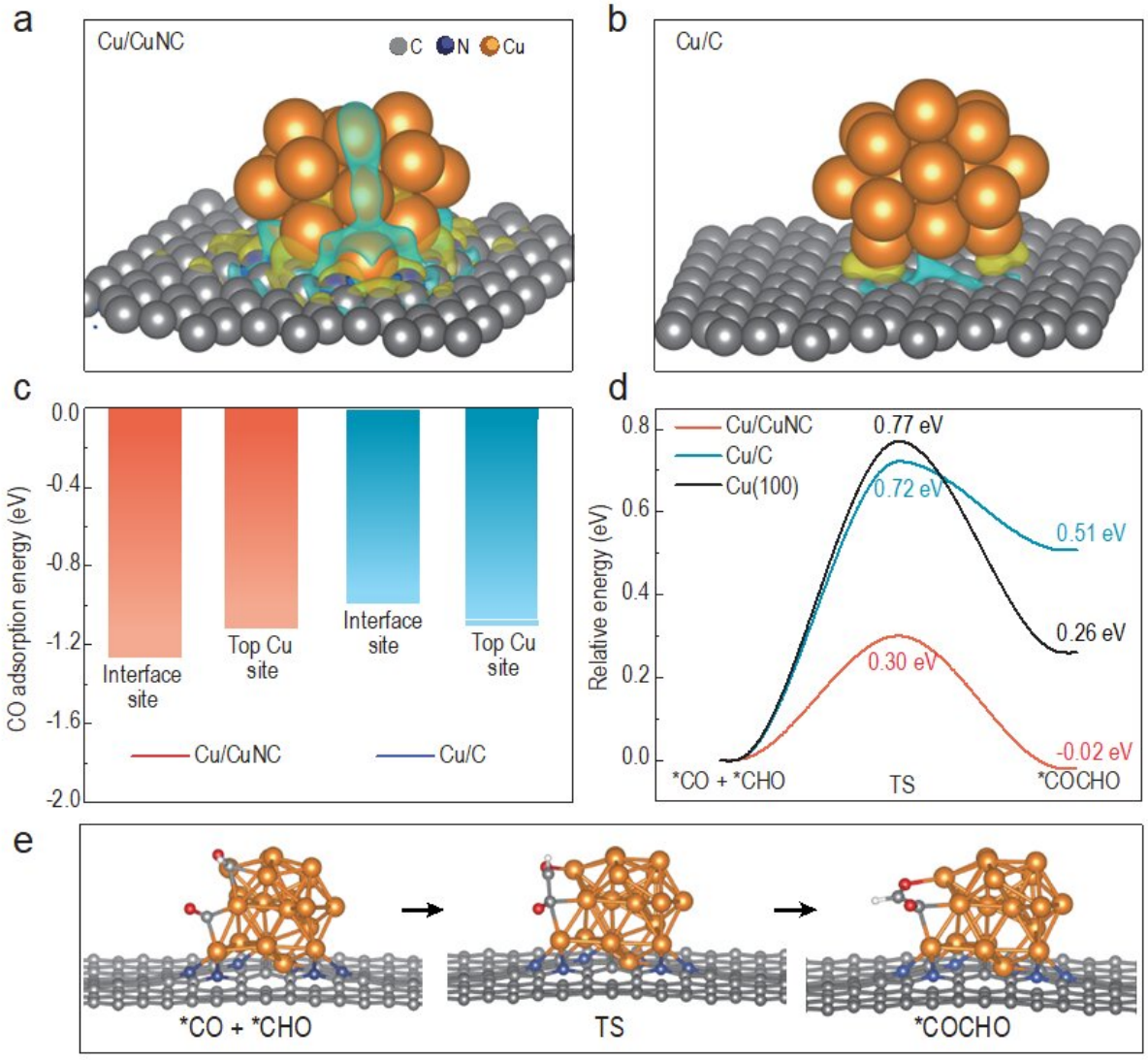
Cu/CuNC dual-site interface promotes carbon dioxide electroreduction to ethanol

February 17 2023



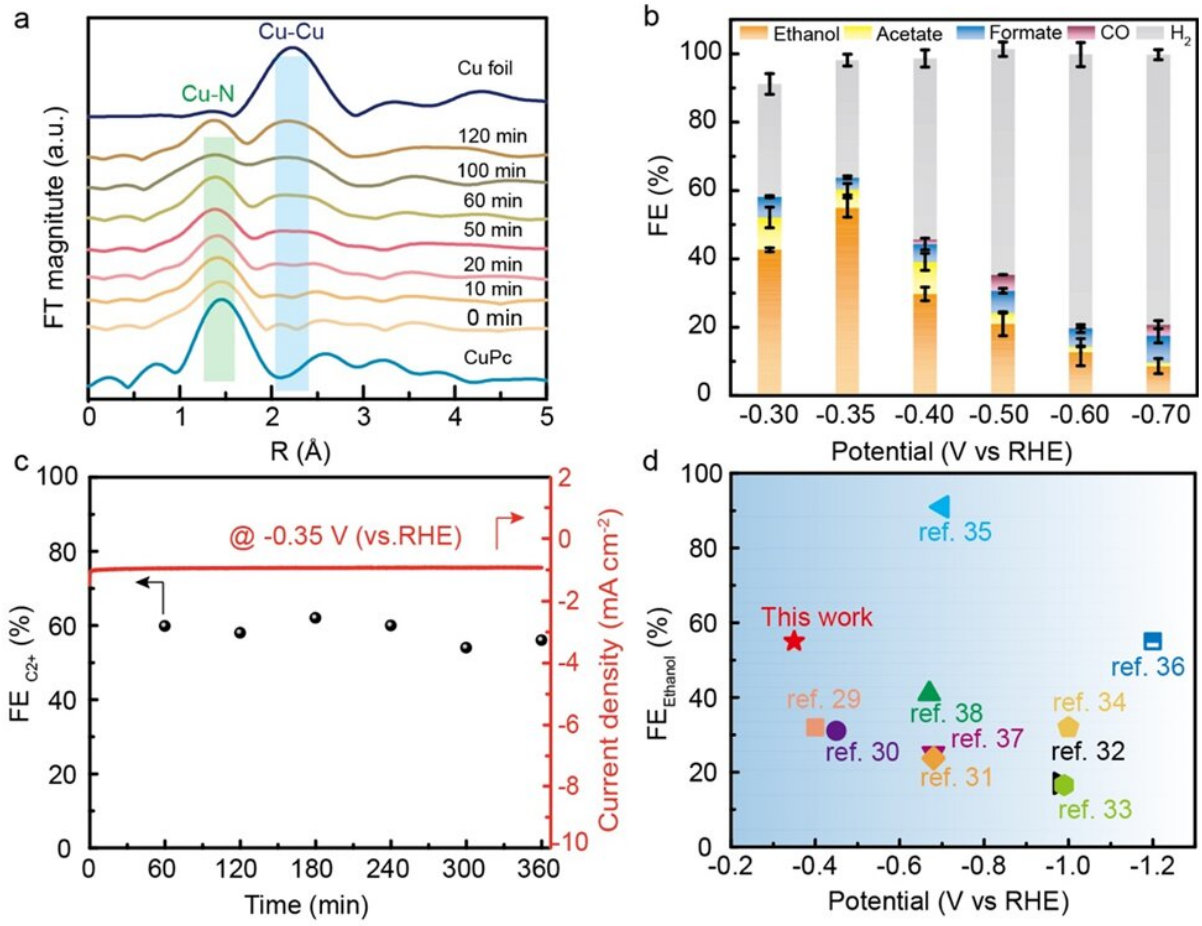
(a-b) Charge density difference map, (c) CO adsorption energy, (d) C-C coupling barriers, and (e) C-C coupling process on different interface sites.

Credit: Science China Press

Reducing the energy consumption is one of requirements for scalable electrochemical energy conversion and electrosynthesis, including electrochemical reduction of CO_2 (ECR) into chemicals.

This study, published in the journal *National Science Review* and led by Prof. Jin-Song Hu (Institute of Chemistry, Chinese Academy of Sciences) and Prof. Jinlan Wang (School of Physics, Southeast University), aims at reducing the overpotential for ECR. The theoretical calculation results were firstly performed, suggesting that the asymmetric electronic structure on the Cu/CuNC interface could significantly enhance the adsorption of *CO intermediate and reduce the reaction energy barrier of the C-C coupling, thereby improving the selectivity of the ethanol at a low overpotential.

The researchers subsequently synthesized such a catalyst with a high density of Cu/CuNC interfacial sites by the in-situ electrochemical reduction of highly loaded CuNC SACs. Ex-situ spectroscopic characterization results evidenced that the nano-sized Cu nanoparticles (~3.6 nm) were formed and surrounded by nitrogen (N).



(a) Operando Cu K edge EXAFS spectra for ER-Cu/CuNC under different electrochemical reduction time at -0.30 V; (b) Potential-dependent FEs for different products, (c) Long-term durability at -0.35 V; (d) Performance comparison. Credit: Science China Press

In-situ spectroscopic characterization results revealed the formation process of the Cu/CuNC interfacial sites and the coexistence of zero-valence Cu and Cu-N-C sites. The ECR tests showed that the ER-Cu/CuNC catalyst exhibited an excellent Faradaic efficiency of 60.3% for C_{2+} (55% for $FE_{ethanol}$) at a low potential of -0.35 V vs. RHE, which is better than most reported Cu-based catalysts.

In addition, the systematical control experiments indicated that the catalysts without Cu/CuNC interfacial sites delivered a negligible ethanol production rate, corroborating the critical role of the Cu/CuNC interfacial sites in promoting C-C coupling at low overpotential. These findings provided new insights and attractive approaches to creating multisite interface as highly efficient catalytic centers for promoting ECR to C_{2+} products at low energy cost.

More information: Yan Yang et al, In-situ Constructed Cu/CuNC Interfaces for Low-Overpotential Reduction of CO2 to Ethanol, *National Science Review* (2022). DOI: 10.1093/nsr/nwac248

Provided by Science China Press