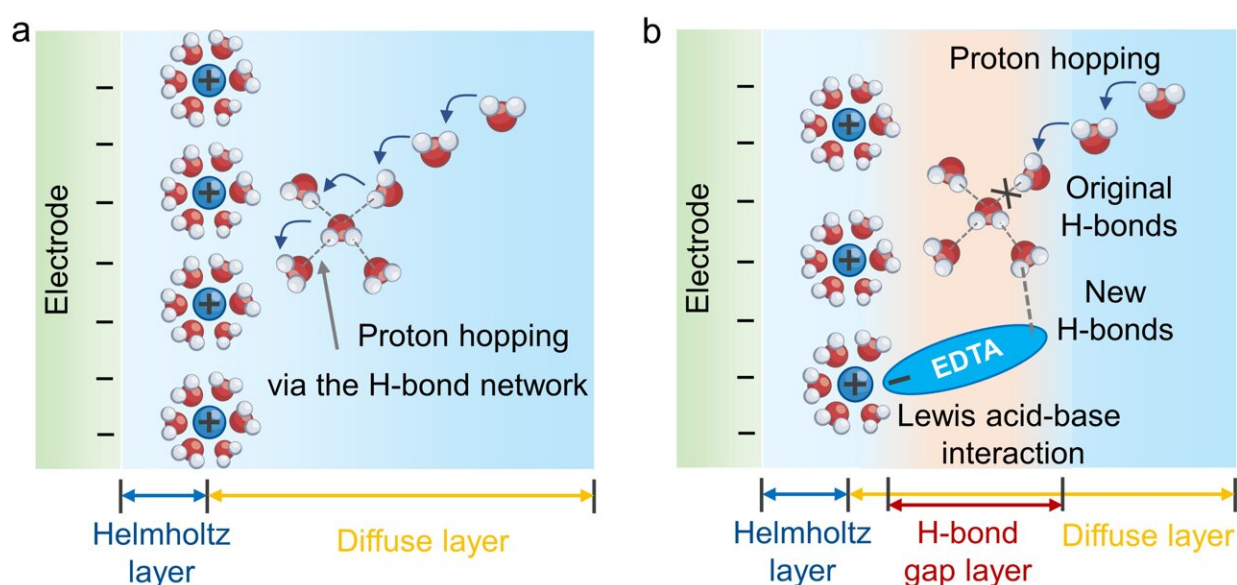


Lewis-base ligand optimized electrolyte composition enhances CO₂ electrolysis performance

August 14 2024



(a) Schematic of interfacial H-bond network for EDTA-free electrolyte. (b) Schematic of interfacial H-bond network and the proposed regulation mechanism for EDTA-containing electrolyte. Credit: Science China Press

The electrode-electrolyte interface where electrocatalytic reactions occur, buried between solid-catalysts and electrolytes, involves complicated processes of electron transfer and mass diffusion under an applied electric field. Understanding the interfacial organization and

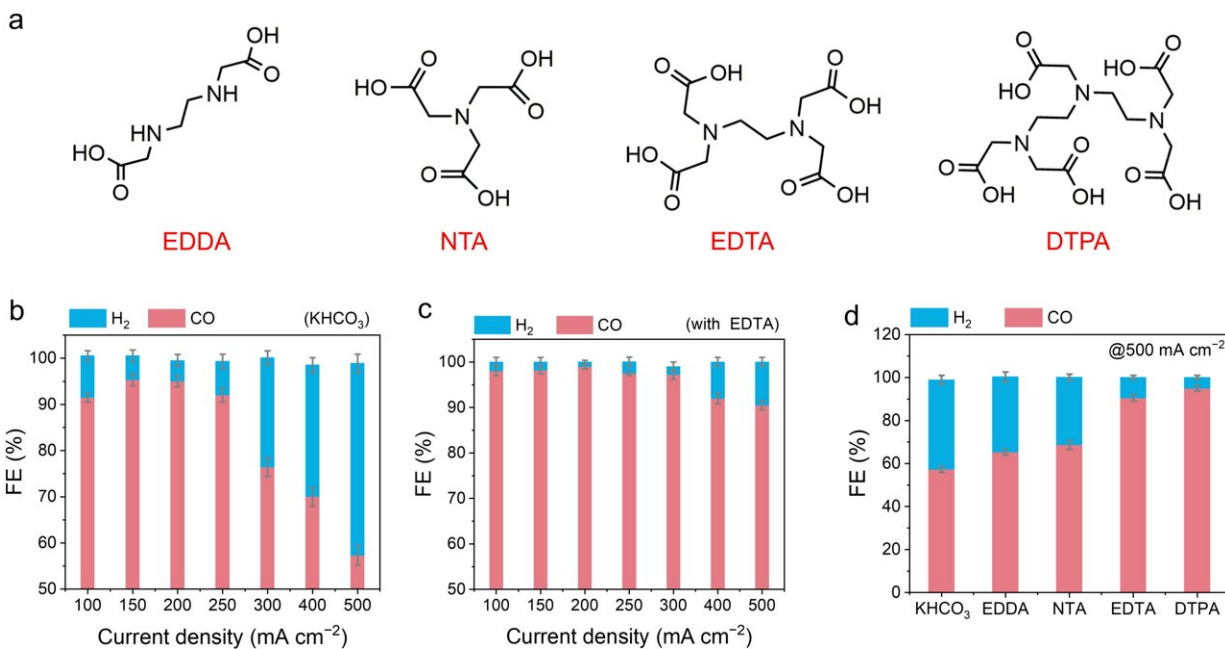
possible interfacial interactions, such as those between the electrocatalysts and electrolytes or among electrolyte components, is essential for improving electrochemical performance via the co-optimization of electrocatalysts and electrolytes.

Recently, Prof. Hongliang Jiang, Prof. Cheng Lian and Prof. Chunzhong Li from East China University of Science and Technology [published](#) a research article titled "Lewis-base ligand-reshaped interfacial hydrogen-bond network boosts CO₂ [electrolysis](#)" in the journal *National Science Review*.

This study proposes a strategy to regulate the electrode-electrolyte interface using Lewis-base ligand molecules. It involves adding trace amounts of ethylenediaminetetraacetic acid molecules and similar ligands as electrolyte additives. In situ infrared and [ab initio](#) molecular dynamics calculations reveal the dynamic changes of ethylenediaminetetraacetic acid ligands at the electrochemical interface and their role in catalyzing CO₂ reduction.

The Lewis-base ligands reconstruct the cation solvation shell through Lewis acid-base interactions and reshape the interface hydrogen-bond network by forming an H-bond gap layer. This strategy can be further extended to a series of commercial catalysts.

This study not only proposes a strategy of Lewis base ligand regulation of catalytic interfaces, but also elucidates the mechanism of Lewis base ligands in CO₂ electrolysis, providing new insights into the interactions of electrolyte components in the electric double layer, and offering a new framework for understanding the organization of complex electrochemical interfaces.



(a) Structural formulae of EDDA, NTA, EDTA, and DTPA. (b) Faradaic efficiency of H₂ and CO at various current densities in 1 M KHCO₃ electrolytes. (c) Faradaic efficiency of H₂ and CO at various current densities in 1 M KHCO₃ electrolytes with 5 mM EDTA. (d) Faradaic efficiency of H₂ and CO at 500 mA cm⁻² in 1 M KHCO₃ electrolytes without and with different Lewis base molecules. Credit: Science China Press

More information: Wangxin Ge et al, Lewis-base ligand-resaped interfacial hydrogen-bond network boosts CO₂ electrolysis, *National Science Review* (2024). [DOI: 10.1093/nsr/nwae218](https://doi.org/10.1093/nsr/nwae218)

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