

Literature Review Summary

Qiang Li*

Department of Quantum Chemistry, University of Bigbro, China

E-mail: lqcata@gmail.com

Abstract

NRR

Machine Learning Accelerated Screening Advanced Single-Atom Anchored MXenes Electrocatalyst for Nitrogen Fixation^{1PDF} ML_NRR_ACS_Catal_Fu_2025.pdf

Tiara Ni Clusters for Electrocatalytic Nitrate Reduction to Ammonia with 97% Faradaic Efficiency^{2PDF} NRR_JACS_Gu_2025.pdf

Selective Mass Accumulation at the Metal-Polymer Bridging Interface for Efficient Nitrate Electroreduction to Ammonia and Zn-Nitrate Batteries^{3PDF} NRR_JACS_Chao_2025.pdf

Isolated Copper Atoms Boost *NO₃ Adsorption and Active Hydrogen Retention over Zinc Oxide for Ammonia Electrosynthesis at Ampere-Level Current Densities^{4PDF} NRR_JACS_Chen_2025.pdf

CO2RR

Enhancing CO₂ Electroreduction to Ethylene in Acidic Solution by Optimizing Cation Configuration on the Cu Surface^{5PDF} ML_CO2RR_JACS_Han_2025.pdf

Mechanism of Potential-Dependent CO₂ Reduction and H₂ Evolution during Electrocatalytic CO₂ Process^{6PDF} CO2RR_ACS Catal_Fu_2025.pdf

Active Sites under Electronic Effect Are More Sensitive to Microenvironment in CO₂ Electroreduction^{7PDF} CO2RR_JACS_Buonsanti_2025.pdf

Competitive Carbonate Binding Hinders Electrochemical CO₂ Reduction to CO on Cu Surfaces at Low Overpotentials^{8PDF} CO2RR_JACS_Lian_2025.pdf

Ammonium Cation-Promoted CO₂ Electroreduction on Au in Acidic Media^{9PDF} CO2RR_JACS_Shi_2025.pdf

Local Coordination Environment-Driven Structural Dynamics of Single-Atom Copper and the CO₂ Electroreduction Pathway^{10PDF} CO2RR_JACS_Lu_2025.pdf

Excess Cations Alter *CO Intermediate Configuration and Product Selectivity of Cu in Acidic Electrochemical CO₂ Reduction Reaction^{11PDF} CO2RR_JACS_Hwang_2025.pdf

Engineering the Coordination Environment of Metal Centers for Selective and High-Current CO₂ Electromethanation^{12PDF} CO2RR_JACS_Zhu_2025.pdf

Identification of Active Regions in a Catalyst Layer on a Gas Diffusion Electrode in the Electroreduction of CO₂^{13PDF} CO2RR_JACS_Sun_2025.pdf

Hydrophobic Cation-Immobilized Covalent Organic Frameworks Enable Selective and Stable Electrosynthesis of Ethylene from CO₂^{14PDF} CO2RR_JACS_Qiang_2025.pdf

Enhanced Nanoconfinement of Copper-Organic Interfaces within Phthalocyanine Frameworks for Selective Electroreduction of CO to Acetate^{15PDF} CORR_JACS_Yang_2025.pdf

OER and HER

A General Machine-Learning Framework for High-Throughput Screening for Stable and Efficient RuO₂-Based Acidic Oxygen Evolution Reaction Catalysts^{16PDF} ML_OER_JACS_Li_2025.pdf

Accelerating Nitrate Electroreduction to Ammonia via Metal-Support Interactions in Ni-WS₂ Catalysts^{17PDF} NRR_JACS_Liu_2025.pdf

Single Atom Engineering for Electrocatalysis: Fundamentals and Applications^{18PDF} ML_OER_ACSCatal_Urso_2025.pdf

References

- (1) Fu, J.; Dong, J.; Si, R.; Sun, K.; Zhang, J.; Li, M.; Yu, N.; Zhang, B.; Humphrey, M. G.; Fu, Q.; Huang, J. Machine-Learning Accelerated Electrocatalyst Design for Nitrogen Reduction Reaction. *ACS Catalysis* **2025**, *15*, 13534–13548.
- (2) Gu, X.; Zhang, J.; Guo, S.; Zhang, Y.; Xu, L.; Jin, R.; Li, G. Tiara Ni Clusters for Electrocatalytic Nitrate Reduction to Ammonia with 97% Faradaic Efficiency. *Journal of the American Chemical Society* **2025**, *147*, 22785–22795.
- (3) Chao, G. et al. Selective Mass Accumulation at the Metal-Polymer Bridging Interface for Efficient Nitrate Electroreduction to Ammonia and Zn-Nitrate Batteries. *Journal of the American Chemical Society* **2025**, *147*, 21432–21442.
- (4) Chen, Z.; Zhao, Y.; Huang, H.; Liu, G.; Zhang, H.; Yan, Y.; Li, H.; Liu, L.; Liu, M.; Wang, D.; Zeng, J. Isolated Copper Atoms Boost *NO₃ Adsorption and Active Hydrogen Retention over Zinc Oxide for Ammonia Electrosynthesis at Ampere-Level Current Densities. *Journal of the American Chemical Society* **2025**, *147*, 18737–18746.

- (5) Han, B. et al. Enhancing CO₂ Electroreduction to Ethylene in Acidic Solution by Optimizing Cation Configuration on the Cu Surface. *Journal of the American Chemical Society* **2025**, *147*, 25584–25591.
- (6) Fu, J.; Dong, J.; Si, R.; Sun, K.; Zhang, J.; Li, M.; Yu, N.; Zhang, B.; Humphrey, M. G.; Fu, Q.; Huang, J. Mechanism of Potential-Dependent CO₂ Reduction and H₂ Evolution during Electrocatalytic CO₂ Process. *ACS Catalysis* **2025**, *15*, 13507–13515.
- (7) Albertini, P. P.; Calderon Mora, J.; Guskova, M.; Rodlamul, P.; Hicks, N.; Leemans, J.; Loidice, A.; Buonsanti, R. Active Sites under Electronic Effect Are More Sensitive to Microenvironment in CO₂ Electroreduction. *Journal of the American Chemical Society* **2025**, *147*, 25517–25526.
- (8) Meng, J.; Freeze, J.; Nowack, L.; Li, C.; Wang, H.; Abruña, H. D.; Willard, A. P.; Batista, V. S.; Lian, T. Competitive Carbonate Binding Hinders Electrochemical CO₂ Reduction to CO on Cu Surfaces at Low Overpotentials. *Journal of the American Chemical Society* **2025**, *147*, 25361–25371.
- (9) Shi, K.; Janisch, J.; Ren, Z.; Meng, Z.; Israel, D.; Le, D.; Kaden, W. E.; Rahman, T. S.; Feng, X. Ammonium Cation-Promoted CO₂ Electroreduction on Au in Acidic Media. *Journal of the American Chemical Society* **2025**, *147*, 23277–23285.
- (10) Lu, T.; Shi, G.; Liu, Y.; Luo, X.; Shen, Y.; Chang, M.; Wu, Y.; Gao, X.; Wu, J.; Li, Y.; Wang, Y.; Zhang, L. Local Coordination Environment-Driven Structural Dynamics of Single-Atom Copper and the CO₂ Electroreduction Pathway. *Journal of the American Chemical Society* **2025**, *147*, 26425–26436.
- (11) Yoo, S.; Park, S.; Son, J.; Kim, J.; Shin, H.; Hwang, Y. Excess Cations Alter *CO Intermediate Configuration and Product Selectivity of Cu in Acidic Electrochemical CO₂ Reduction Reaction. *Journal of the American Chemical Society* **2025**, *147*, 12996–13007.

- (12) Zhu, C.; Wang, D.; Zeng, L.; Feng, G.; Liang, Y.; Zheng, W.; Lin, W.; Peng, X.; Liu, Z.; Sang, X.; Yang, B.; Li, Z.; Zhang, Q.; Lei, L.; Hou, Y. Engineering the Coordination Environment of Metal Centers for Selective and High-Current CO₂ Electromethanation. *Journal of the American Chemical Society* **2025**, *147*, 26185–26194.
- (13) Sun, Q.; Zheng, Y.; Wang, J.; Ye, Y.; Fu, L.; Xiong, H.; Song, H.; Chang, X.; Xu, B. Identification of Active Regions in a Catalyst Layer on a Gas Diffusion Electrode in the Electroreduction of CO₂. *Journal of the American Chemical Society* **2025**, *147*, 21621–21628.
- (14) Qian, Z.; Liu, Y.; Lin, Z.; Ye, N.; Tan, Y.; Liu, F.; Gu, Y.; Huang, Q.; Guo, H.; Luo, M.; Guo, S. Hydrophobic Cation-Immobilized Covalent Organic Frameworks Enable Selective and Stable Electrosynthesis of Ethylene from CO₂. *Journal of the American Chemical Society* **2025**, *147*, 26425–26436.
- (15) Yang, Q.; Chen, Y.; Liu, N.; Li, S.; Chen, M.; Zheng, W.; Fu, Y.; Han, J.; Rodriguez, R. D.; Hou, Y.; Zhang, T. Enhanced Nanoconfinement of Copper-Organic Interfaces within Phthalocyanine Frameworks for Selective Electroreduction of CO to Acetate. *Journal of the American Chemical Society* **2025**, *147*, 22132–22140.
- (16) Shang, Z.; Zhao, S.; Dang, Q.; Wang, F.; Sun, X.; Li, H. A General Machine-Learning Framework for High-Throughput Screening for Stable and Efficient RuO₂-Based Acidic Oxygen Evolution Reaction Catalysts. *ACS Catalysis* **2025**, *15*, 12835–12847.
- (17) Lv, J.; Yang, Q.; Liang, T.; Sun, X.; Rong, W.; Dai, Q.; Gao, Y.; Wang, L.; Xu, X.; Liu, Y. Accelerating Nitrate Electroreduction to Ammonia via Metal-Support Interactions in Ni–WS₂ Catalysts. *Journal of the American Chemical Society* **2025**, *147*, 25361–25371.
- (18) Urso, M.; Ju, X.; Nittoor Veedu, R.; Lee, H.; Zaoralova, D.; others Single-Atom Engi-

neering for Electrocatalysis: Fundamentals and Applications. *ACS Catalysis* **2025**, *15*, 11617–11663.