

# Mechanism of CO<sub>2</sub> Reduction by Ruthenium Electrocatalysts

## Scientific Achievement

Key mechanistic details of ruthenium-catalyzed CO<sub>2</sub> electroreduction were elucidated via theory and experiment.

## Significance and Impact

- Organometallic Ru catalysts supported by N-heterocyclic carbene ligands are leading catalysts for tunable CO/H<sub>2</sub> generation.
- Density Functional Theory (DFT) and experimental studies support the importance of a cis/trans isomerization during the catalytic cycle, guiding future catalyst designs.

## Research Details

- DFT predicted intermediate energetics.
- Both isomers of nitrile and CO complexes were synthesized in the lab.
- Electrochemistry corroborated DFT.

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Work was performed at UNC-CH and Brookhaven National Laboratory

