Atomically-Precise Cu Nanoclusters to Electrochemically Reduce CO2 Into Valuable Chemicals

Almutairi, Mesk (School: Fatima Bint Almonthir)

Global carbon dioxide (CO2) emissions, exceeding 37 billion tons annually, are intensifying environmental crises and threatening public safety. Electrochemical CO2 reduction reaction (eCO2RR) offers an optimistic approach by converting CO2 into valuable products, supporting a circular carbon economy. While Cu nanoclusters (NCs) have emerged as promising catalysts due to their cost-effectiveness and atomic precision, challenges remain in selectivity and efficiency at high current densities. This study introduces two novel Cu NCs and investigates their catalytic performance targeting useful hydrocarbons under industrially relevant conditions. Cu10(CF3Pyrazole)8 and Cu6((CF3)2Pyrazole)6Cl4, were synthesized with N-donor ligands to enhance CO2 adsorption and fluoro groups for hydrophobicity, suppressing the competing hydrogen evolution reaction (HER). Each catalyst was mixed with 10% Nafion as a binder and spray-coated onto a Gas diffusion electrode (GDE). The eCO2RR occurred in a flow cell at 150 mA/cm2, with product analysis performed via 1H NMR and GC. Cu6((CF3)2Pyz)6Cl4 initially yielded 7% Faradaic Efficiency (FE) for ethylene, which doubled to 14% upon increasing the 10% Nafion amount from 40 µL to 80 µL. As for Cu10(CF3Pyz)8, it produced propanol, marking the first reported NCs to generate this C3 hydrocarbon. These catalysts, with their higher scalability, simplicity for improving ethylene selectivity, and capability of producing complex compounds, outperform existing Cu NCs. The production of ethylene, the foundation of most high-demand petrochemicals, through an effective sustainable pathway could significantly lower reliance on fossil fuels and the carbon footprint of major industries.

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