

Potassium-promoted Selective CO₂ to Methanol Conversion over a Cu_xO/Cu(111) Model Surface

Scientific Achievement

Researchers revealed that potassium (K) deposited on a Cu_xO/Cu(111) model surface facilitated the conversion of CO₂ and described mechanistic processes that tune product selectivity from CO to methanol, based on combined density functional theory (DFT) and kinetic Monte Carlo (KMC) simulation.

Significance and Impact

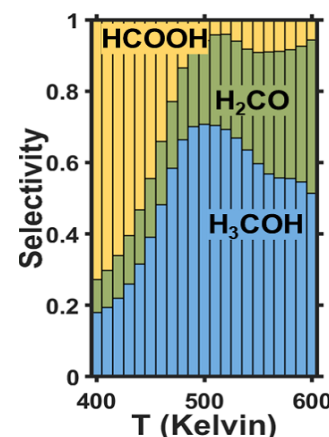
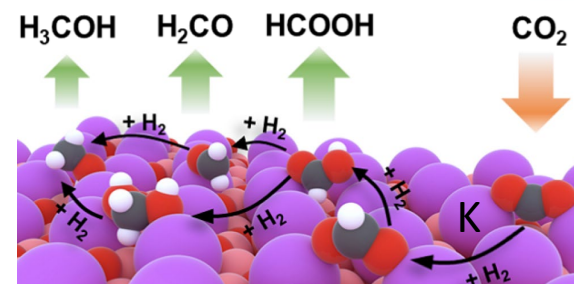
Direct conversion of CO₂ to methanol is a challenge in industrial catalysis. Alkali promotion of metal-oxide catalysts for this and related reactions is important to improve performance. The new mechanistic understanding for alkali-based catalysts provides design rules linking alkali-surface electrostatic interaction and alkali-mediated charge transfer to reactive binding of reactants and intermediates and catalytic activity/selectivity.

Research Details

DFT computation showed deposited K⁺ ions play multifunctional roles: an active center for selective tuning in binding of reaction intermediates, an accelerator for charge transfer, and a mediator for electron tunneling. Both DFT calculations and KMC simulations predict the K opens a new *H₂C(OH)₂-mediated formate pathway for selective CO₂ conversion to methanol and suppresses the CO production via reverse-water-gas-shift reaction.

Sensitivity analysis predicts that stabilization of formic acid intermediates while destabilizing the formate intermediates will improve CO₂ conversion and methanol selectivity.

Wenjie Liao, and Ping Liu, *ACS Catal.* 2020, 10, 5723-5733 (Cover).



Theory shows potassium (K) sites are multifunctional and open a new pathway enabling the temperature-dependent selective conversion of CO₂ to methanol.