

Structure-Activity Relationships of Cu-ZrO₂ Catalysts for CO₂ Hydrogenation to Methanol: Interaction Effects and Reaction Mechanism

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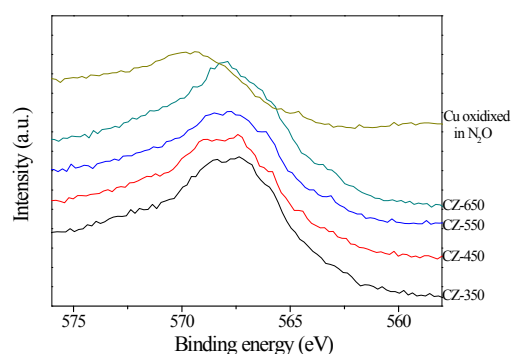


Figure S1. The change in the Cu L3VV Auger line for the reduced CZ catalyst and Cu oxidized in N₂O

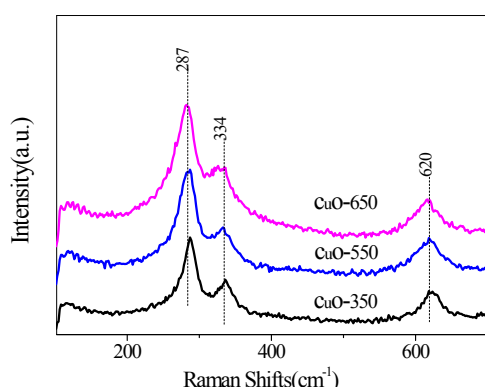


Figure S2. Raman spectra of various CuO calcinated at 350, 550 and 650 °C.

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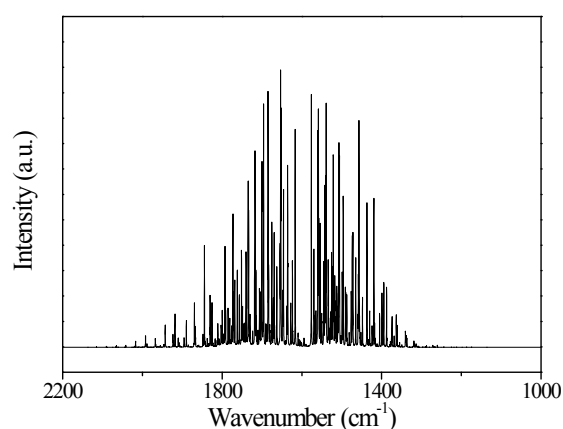


Figure S3. In situ DRIFT spectra of H₂O (1000ppm)

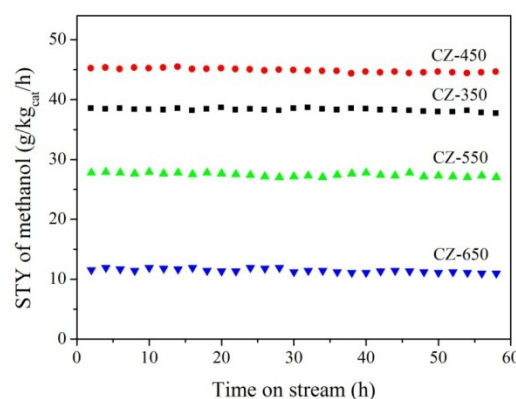


Figure S4. Space-time yield (STY) of methanol as a function of time-on-stream over CZ-350, CZ-450, CZ-550 and CZ-650. Reaction conditions: T=220 °C, CO₂:H₂=1:3, P=3.0 MPa, GHSV=3600 h⁻¹.

Stability is a key factor in determining whether the Cu/ZrO₂ materials can be used as methanol synthesis catalyst for CO₂ hydrogenation reaction in industrial production. Figure S4 shows the STY versus the time-on-stream of methanol over four catalysts: CZ-350, CZ-450, CZ-550 and CZ-650. It was found that the STY for methanol decreased by less than 3% from its initially stabilized values. It was obvious that the CZ catalysts exhibited a stable catalytic performance for the whole test period.