



Operando Identification of Dynamic ZrO_x–Cu Perimeter Sites during Low-Temperature CO₂ Hydrogenation

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ABSTRACT

The catalytic conversion of CO₂ to methanol over Cu-based catalysts is strongly influenced by oxide–metal interfacial structures, yet the dynamic evolution of these sites under reaction conditions remains insufficiently understood. Herein, a series of ZrO_x-modified Cu catalysts with Zr/Cu atomic ratios from 0.015 to 0.120 were prepared by controlled surface deposition and evaluated for CO₂ hydrogenation at 220–260 °C and 3.0 MPa. Operando diffuse reflectance infrared Fourier-transform spectroscopy, quasi in situ X-ray photoelectron spectroscopy, H₂ temperature-programmed reduction, and Cu K-edge X-ray absorption spectroscopy were combined with kinetic measurements to determine the active interfacial motifs. The catalyst with a Zr/Cu ratio of 0.065 delivered the highest methanol space–time yield of 412.7 gMeOH kgcat^{−1} h^{−1} at 240 °C, with CO₂ conversion of 13.4% and methanol selectivity of 71.9%. Compared with unmodified Cu, the apparent activation energy decreased from 86.5 to 58.2 kJ mol^{−1}, while the methanol formation rate increased by a factor of 3.6. Operando spectra show that bidentate formate bands at 1584 and 1367 cm^{−1} intensified rapidly on ZrO_x-rich perimeter sites and were subsequently converted into methoxy species at 1048 cm^{−1}. Isotopic switching using D₂ revealed a kinetic isotope effect of 2.3, indicating that hydrogen addition to surface formate remains a kinetically relevant step. Long-term testing for 120 h showed only 6.8% activity loss, which was attributed to partial aggregation of surface ZrO_x domains rather than Cu sintering. This study demonstrates that highly dispersed ZrO_x–Cu perimeters act as dynamic catalytic ensembles and that their structural retention is essential for maintaining methanol selectivity under low-temperature CO₂ hydrogenation conditions.

1. Introduction

CO₂ hydrogenation to methanol provides a promising route for coupling captured carbon with renewable H₂ and converting them into a transportable chemical product. Methanol is widely used as a fuel, an energy carrier, and a feedstock for the production of olefins, formaldehyde, and other commodity chemicals. The reaction, however, remains kinetically demanding because the high thermodynamic stability of CO₂ requires sequential activation and hydrogen-transfer steps before the C–O framework can be converted into methanol. Methanol synthesis also competes with the reverse water–gas shift reaction, which produces CO and becomes increasingly important at elevated temperatures. Cu-based catalysts are among the most extensively studied materials for this reaction because Cu can activate H₂ and promote the hydrogenation of adsorbed carbon-containing

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intermediates under relatively moderate conditions. Their catalytic behavior is highly sensitive to Cu particle size, oxidation state, surface coordination, and interaction with neighboring oxide phases. Operando studies of Cu–Zn catalysts have shown that Cu oxidation state, Zn distribution, and metal–oxide interfacial structure respond continuously to changes in temperature, pressure, and reaction atmosphere (Ughade et al., 2025; You, 2026). Related behavior has also been observed in Cu catalysts promoted with Zn-, Ga-, Mg-, and Ce-containing oxides, where highly dispersed oxide domains, oxygen vacancies, Cu⁺ species, and surface hydroxyl groups can alter CO₂ adsorption, hydrogen transfer, and methanol selectivity (Jiao et al., 2026a; Todaro et al., 2026). The catalytically relevant Cu–oxide interface should therefore be considered a reaction-dependent structure whose population and chemical state may vary substantially under working conditions.

Among oxide promoters, ZrO₂ is particularly attractive because it combines thermal stability with acid–base functionality, surface hydroxyl groups, and defect sites capable of binding and activating CO₂. Depositing highly dispersed ZrO_x species directly onto Cu creates an inverse catalyst geometry in which a large fraction of the oxide is located close to metallic Cu. This configuration can generate interfacial ensembles that are structurally different from those found in conventional Cu/ZrO₂ catalysts. Recent atomistic modeling of inverse ZrO₂/Cu has further shown that the catalytic surface contains an ensemble of structurally distinct interfacial configurations with markedly different reactivities, and that changes in the population of these configurations can influence both methanol formation and catalyst deactivation (Yang et al., 2026a). This result is important because it suggests that describing the catalyst using a single idealized Cu–ZrO_x active site may overlook the structural heterogeneity present under reaction conditions. Experimental studies similarly report that inverse ZrO_x/Cu catalysts can achieve higher methanol formation rates than conventional Cu/ZrO₂ materials, particularly when highly dispersed ZrO_x domains generate a high density of oxide–metal boundaries (Lee et al., 2026; Liang et al., 2026). The enhancement cannot be attributed simply to the total amount of Zr. ZrO_x coverage determines how much interfacial perimeter is created and how much Cu surface remains available for H₂ dissociation and hydrogen transfer. Insufficient coverage provides only a limited number of Cu–ZrO_x boundary sites, whereas excessive deposition can decrease exposed Cu area, promote the formation of larger oxide domains, and alter the accessibility of interfacial sites. An optimum coverage is therefore expected to reflect a balance between interfacial site generation and preservation of the complementary functions of Cu and ZrO_x. The chemical role of ZrO_x is closely associated with the adsorption and transformation of oxygen-containing C₁ intermediates. Surface hydroxyls, Lewis acid–base pairs, and oxygen defects on ZrO₂ can stabilize carbonate, bicarbonate, formate, and methoxy species formed during CO₂ hydrogenation. Formate is particularly prominent in infrared spectra and has consequently been incorporated into many proposed mechanisms for methanol synthesis over Cu/ZrO₂-related catalysts. Its high surface concentration, however, does not necessarily indicate a high reaction flux through the formate pathway. Time-resolved infrared measurements have demonstrated that formate populations may contain species with substantially different kinetic behavior: some undergo further hydrogenation toward methoxy, whereas others remain strongly bound to the oxide surface and contribute little to methanol production. Surface and kinetic studies have also identified hydrogen-transfer reactions involving adsorbed formate as potentially important kinetic constraints under specific catalyst structures and reaction conditions (Baghdady et al., 2025; Chen et al., 2025). At the same time, the stability and reactivity of formate depend strongly on the local Zr coordination environment, surface termination, hydroxyl coverage, and crystallographic structure of ZrO₂ (Kim et al., 2026; Liang et al., 2025). The observation of an intense formate band alone is therefore insufficient to establish that the detected species is a productive reaction intermediate. Mechanistic assignment requires a direct connection between

intermediate dynamics and measurable methanol formation rates. This distinction becomes particularly important when comparing catalysts with different ZrO_x coverages. Increasing Zr loading can increase the number of CO_2 adsorption sites and the apparent concentration of formate without necessarily increasing the number of productive Cu– ZrO_x perimeter sites. Large ZrO_x domains may stabilize spectator formates more strongly than isolated or highly dispersed interfacial species, while simultaneous coverage of Cu may reduce the surface available for H_2 dissociation. Changes in infrared intensity can therefore reflect differences in adsorption capacity, intermediate residence time, or surface site density rather than changes in catalytic turnover (Du, 2025; Hadjiivanov et al., 2026). Isotopic switching provides a useful means of separating these effects because the replacement of H_2 by D_2 probes the exchange and hydrogenation behavior of surface intermediates under reaction conditions. When combined with kinetic measurements, the decay and replacement of formate- and methoxy-related bands can be compared directly with methanol production. Such analysis can determine whether an accumulated intermediate responds on a timescale compatible with catalytic turnover and whether the hydrogen-transfer step associated with that intermediate contributes significantly to the observed rate. A further complication is that ZrO_x modification can influence the Cu phase itself. The introduction of zirconium oxide may change Cu reducibility, stabilize partially oxidized Cu species near the interface, modify Cu coordination, or alter the resistance of Cu particles to sintering. Cu^0 and interfacial Cu^+ species may perform different functions in H_2 activation and stabilization of oxygenated intermediates, making the Cu^0/Cu^+ distribution an additional variable that must be separated from the effect of ZrO_x coverage. Conventional ex situ characterization provides only limited information in this respect. X-ray diffraction can identify crystalline phases and estimate particle dimensions but is relatively insensitive to highly dispersed or amorphous ZrO_x . Ex situ TEM provides local structural information, although the configuration observed after reaction may differ from that under the reacting gas mixture. Similarly, conventional XPS records the surface after removal from the catalytic environment and may therefore miss reversible changes in Cu oxidation state and interfacial chemistry (Jiao et al., 2026b; Yang, 2026b). Combining quasi in situ XPS with Cu K-edge X-ray absorption spectroscopy, H_2 temperature-programmed reduction, and operando vibrational spectroscopy offers a more complete description of the electronic, structural, and chemical evolution of the working Cu– ZrO_x interface. Catalyst stability introduces another unresolved aspect of this system. Activity loss during CO_2 hydrogenation over Cu-based catalysts is often attributed to Cu sintering, yet structural changes in the promoter phase may occur on a different timescale. Migration and coalescence of initially dispersed ZrO_x species can decrease the length of the Cu– ZrO_x perimeter even when the average Cu particle size changes only moderately. Such restructuring may also alter the distribution of Cu^+ sites, hydroxyl groups, and adsorption environments for formate and methoxy. Short stability experiments cannot readily distinguish rapid surface equilibration from slower irreversible structural evolution (Mohsen & Allam, 2026; Moss et al., 2025). Longer tests, supported by characterization before and after reaction, are therefore needed to determine whether deactivation originates mainly from Cu particle growth, loss of highly dispersed ZrO_x , changes in oxidation state, or a combination of these processes (Wu et al., 2026). Establishing the dominant deactivation route is particularly important for inverse catalysts because their high initial activity is associated with a large amount of highly dispersed oxide–metal perimeter that may also be structurally vulnerable under hydrothermal reaction conditions. Despite substantial progress, the relationship among ZrO_x coverage, working interfacial structure, intermediate kinetics, and long-term stability remains insufficiently resolved. Comparisons across previous studies are complicated by simultaneous variations in Cu particle size, ZrO_2 phase, synthesis route, surface area, reduction history, and reaction conditions. Zr content is commonly

expressed as a bulk composition even though methanol formation is expected to depend primarily on the amount and structure of ZrO_x exposed at the Cu perimeter. Spectroscopic studies frequently identify formate as a dominant surface intermediate without determining whether its consumption follows the rate of methanol formation, while catalyst stability is often assessed over periods too short to distinguish Cu sintering from the slower restructuring of the ZrO_x phase. The present study addresses these limitations using a controlled series of ZrO_x -modified Cu catalysts with Zr/Cu atomic ratios ranging from 0.015 to 0.120, prepared by controlled surface deposition to systematically vary the extent of the Cu– ZrO_x interface. Operando DRIFTS, quasi in situ XPS, H_2 temperature-programmed reduction, and Cu K-edge X-ray absorption spectroscopy are combined with steady-state kinetics and D_2 switching experiments to determine how ZrO_x coverage affects Cu electronic structure, interfacial site population, formate-to-methoxy conversion, and methanol formation. The relationship between spectroscopically observed intermediate dynamics and kinetic behavior is examined to distinguish productive formate species from strongly adsorbed spectators and to identify the hydrogen-transfer steps most closely associated with catalytic turnover. A 120 h stability experiment is further used to separate changes in Cu particle structure from the evolution of dispersed ZrO_x domains and to establish the structural origin of activity loss. By connecting controlled ZrO_x coverage with perimeter structure, intermediate reactivity, methanol formation rate, and long-term stability, this work aims to provide a quantitative basis for understanding the working Cu– ZrO_x interface and to define design principles for Cu-based methanol synthesis catalysts that combine high interfacial activity with improved structural stability.

2. Materials and Methods

2.1. Catalyst Samples and Reaction Conditions

Seven Cu-based catalysts were prepared with Zr/Cu atomic ratios of 0, 0.015, 0.030, 0.045, 0.065, 0.090, and 0.120. The Zr-free sample was used as the Cu control. Copper powder with an average particle size of 2–5 μm served as the base material. Zr was deposited on the Cu surface by hydrolysis of zirconyl nitrate. Diluted ammonia was added to keep the pH at 8.5. The solids were filtered, washed with deionized water, and dried at 80 $^\circ\text{C}$ for 12 h. They were then heated in N_2 at 300 $^\circ\text{C}$ and reduced in 10 vol% H_2/N_2 at 280 $^\circ\text{C}$. CO_2 hydrogenation was tested in a stainless-steel fixed-bed reactor at 220–260 $^\circ\text{C}$ and 3.0 MPa. The feed contained H_2 , CO_2 , and N_2 at a molar ratio of 72:24:4. The total flow rate was 60 mL min^{-1} , and 150 mg of catalyst was used in each run. Each catalyst was prepared in two separate batches, and each reaction condition was tested three times.

2.2. Experimental Design and Control Tests

The catalyst series was used to study how ZrO_x coverage affects ZrO_x –Cu boundary sites. Unmodified Cu served as the main control. A physical mixture of Cu and ZrO_2 with a Zr/Cu ratio of 0.065 was also tested. This sample was used to compare close surface contact with simple particle mixing. A Cu/ ZrO_2 catalyst prepared by impregnation was included as a second control. It had the same Zr content as the best surface-deposited sample. Before each reaction, the catalyst was reduced in the reactor at 280 $^\circ\text{C}$ for 2 h. Product data were collected after the outlet gas remained stable for at least 90 min. Blank tests were conducted without a catalyst and with pure ZrO_2 . Reaction orders were measured by changing the partial pressures of H_2 and CO_2 while keeping the total flow rate constant. External mass transfer was checked by changing the flow rate from 40 to 80 mL min^{-1} . Internal diffusion was examined using particle sizes of 150–250 and 250–425 μm . No clear change in the mass-based methanol rate was observed within these ranges.

2.3. Structural Measurements and Quality Control

Crystal phases were identified by X-ray diffraction using Cu K α radiation. Surface shape and ZrO $_x$ distribution were examined by transmission electron microscopy and high-angle annular dark-field scanning transmission electron microscopy. The surface states of Cu, Zr, and O were measured by quasi in situ X-ray photoelectron spectroscopy. Reduced and reacted samples were transferred to the analysis chamber without contact with air. Cu K-edge X-ray absorption spectra were collected under reaction gas to measure changes in the Cu oxidation state and local structure. H $_2$ temperature-programmed reduction was carried out from 50 to 500 °C at a heating rate of 10 °C min $^{-1}$. Carbonate, formate, methoxy, and adsorbed CO species were monitored by operando diffuse reflectance infrared Fourier-transform spectroscopy at 3.0 MPa. Reaction products were measured by online gas chromatography. Methanol and other oxygen-containing products were measured with a flame-ionization detector. CO $_2$, CO, H $_2$, and N $_2$ were measured with a thermal-conductivity detector. Certified standards were used for calibration. Data were accepted when the carbon balance was between 95% and 105%. The reactor temperature was kept within ± 1 °C, and the variation among repeated tests was below 5%.

2.4. Data Processing and Kinetic Analysis

Gas concentrations were corrected using N $_2$ as an internal standard. CO $_2$ conversion was calculated as

$$X_{\text{CO}_2}(\%) = \frac{F_{\text{CO}_2,\text{in}} - F_{\text{CO}_2,\text{out}}}{F_{\text{CO}_2,\text{in}}} \times 100,$$

where $F_{\text{CO}_2,\text{in}}$ and $F_{\text{CO}_2,\text{out}}$ are the inlet and outlet molar flow rates of CO $_2$, respectively. Methanol selectivity was calculated on a carbon basis using the outlet flow rates of methanol, CO, and CH $_4$. Methanol space-time yield was expressed as grams of methanol produced per kilogram of catalyst per hour. The apparent activation energy was calculated using the Arrhenius equation:

$$\ln r_{\text{MeOH}} = \ln A - \frac{E_a}{RT},$$

where r_{MeOH} is the methanol formation rate, A is the pre-exponential factor, E_a is the apparent activation energy, R is the gas constant, and T is the reaction temperature. Linear fitting used data obtained below 10% CO $_2$ conversion to reduce heat- and mass-transfer effects. Results are reported as mean values with standard deviations. Differences among the catalysts were examined by one-way analysis of variance followed by Tukey's test. A value of $p < 0.05$ was considered significant.

2.5. Operando, Isotope, and Stability Tests

Operando DRIFTS spectra were collected during CO $_2$ hydrogenation at 240 °C and 3.0 MPa. A background spectrum was recorded after catalyst reduction. Spectra were then collected every minute until the main bands became stable. To study hydrogen addition to surface formate, the feed was changed from H $_2$ /CO $_2$ to D $_2$ /CO $_2$. The total pressure and flow rate were kept constant. The kinetic isotope effect was calculated from the ratio of methanol formation rates under H $_2$ and D $_2$. Step-response tests were also conducted by switching among CO $_2$, H $_2$, and CO $_2$ /H $_2$ feeds. These tests separated CO $_2$ adsorption, formate formation, and later hydrogenation steps. Catalyst stability was tested at 240 °C and 3.0 MPa for 120 h. After the test, XRD, electron microscopy, quasi in situ XPS, and X-ray absorption measurements were repeated. Changes in Cu particle size and ZrO $_x$ domain size were compared to identify the main cause of activity loss.

3. Results and Discussion

3.1. Effect of ZrO_x Coverage on the Cu Surface

The amount of ZrO_x changed the surface structure of the Cu catalysts. At low Zr/Cu ratios, small ZrO_x domains were spread across the Cu surface, and most Cu sites remained exposed. A Zr/Cu ratio of 0.065 produced more ZrO_x -Cu boundary sites without covering much of the Cu surface. Quasi in situ XPS showed a small shift in the Cu binding energy. Cu K-edge spectra showed that Cu remained mainly metallic during the reaction. These results indicate electron transfer between Cu and nearby ZrO_x species. H_2 -TPR also showed that ZrO_x addition made the catalyst easier to reduce. At higher Zr/Cu ratios, the ZrO_x domains became larger and covered more Cu sites. This reduced the number of sites available for H_2 dissociation. The changes in catalyst structure and surface state are shown in Fig. 1. Todaro et al. (2026) also reported that small ZrO_2 domains on Cu formed more active boundary sites than large oxide particles. Their results showed a volcano-shaped relation between ZrO_2 loading and methanol production (Bao et al., 2026a; Phongprueksathat et al., 2026).

3.2. Methanol Production and Reaction Kinetics

Methanol production increased with the Zr/Cu ratio and reached its highest value at 0.065. At 240 °C and 3.0 MPa, this catalyst gave a CO_2 conversion of 13.4%, a methanol selectivity of 71.9%, and a methanol space-time yield of 412.7 gMeOH kgcat⁻¹ h⁻¹. Lower Zr contents produced too few boundary sites for CO_2 adsorption. Higher Zr contents covered part of the Cu surface and limited H_2 activation. The physical mixture and impregnated Cu/ ZrO_2 catalyst also showed lower methanol rates than the surface-deposited sample. This result confirms that close ZrO_x -Cu contact was more important than the total Zr content. The apparent activation energy decreased from 86.5 kJ mol⁻¹ on unmodified Cu to 58.2 kJ mol⁻¹ on the catalyst with a Zr/Cu ratio of 0.065. The methanol formation rate increased by 3.6 times, as shown in Fig. 1. These results indicate that ZrO_x lowered the reaction barrier rather than only increasing CO_2 adsorption. Similar loading effects have been reported for inverse ZrO_2 /Cu catalysts, where moderate oxide coverage gave the highest methanol yield (Goyal et al., 2026; Gu, 2026).

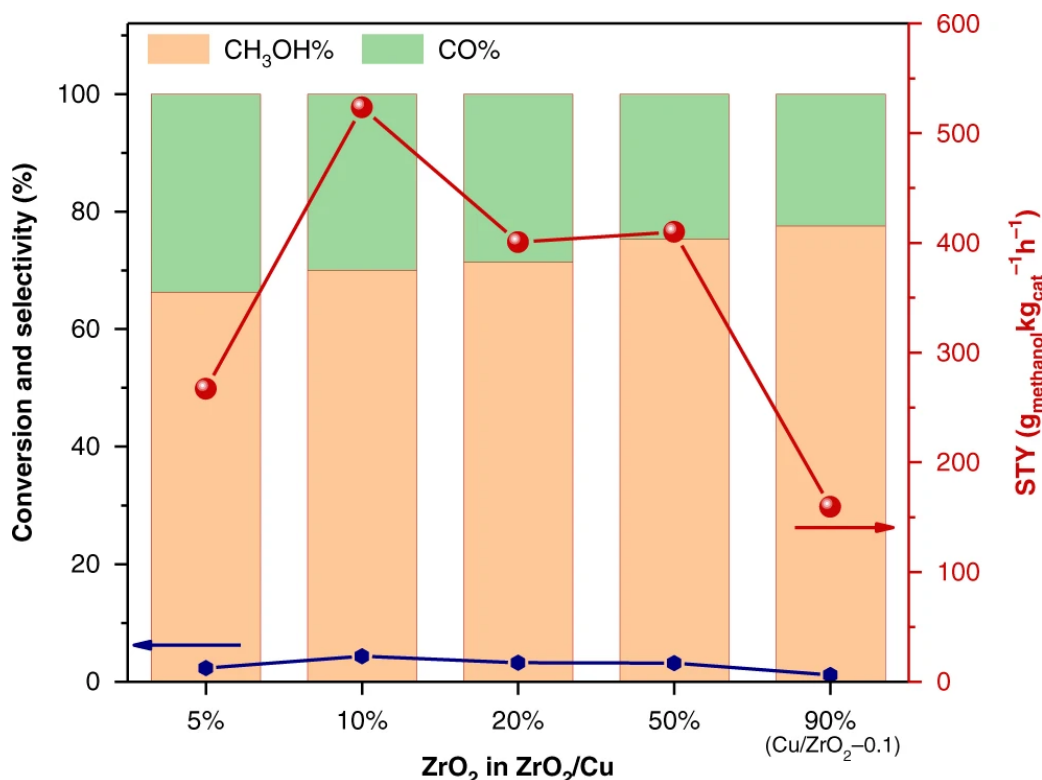


Fig. 1. Effect of the Zr/Cu ratio on catalyst structure, methanol yield, and apparent activation energy.

3.3. Formate Hydrogenation at ZrO_x–Cu Boundaries

Operando DRIFTS detected bidentate formate bands at 1584 and 1367 cm⁻¹ after the CO₂/H₂ feed was introduced. These bands formed faster on the catalyst with a Zr/Cu ratio of 0.065 than on unmodified Cu. A methoxy band later appeared at 1048 cm⁻¹. During the H₂ step-response test, the formate bands decreased while the methoxy band increased, as shown in Fig. 2. This change supports the conversion of formate into methoxy species. Samples with high Zr contents retained strong formate bands, but methoxy formation was slower. Large ZrO_x domains may therefore store formate while limiting its contact with active hydrogen. D₂ switching gave a kinetic isotope effect of 2.3. This result shows that hydrogen addition takes part in a rate-related step. The lower activation energy and isotope effect indicate that the ZrO_x–Cu boundary supports hydrogen transfer to surface formate. Baghdady et al. (2025) also identified formate species with different reaction rates on Cu/ZrO₂. The more active formate species were closely linked to methoxy formation.

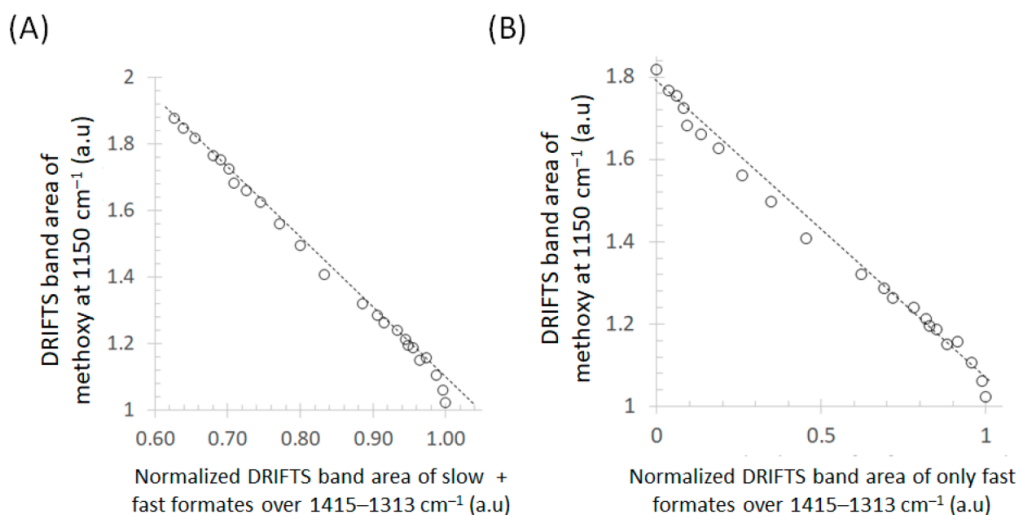


Fig. 2. Changes in formate and methoxy species during methanol formation at $\text{ZrO}_x\text{-Cu}$ interfaces.

3.4. Interface Structure and Catalyst Stability

The operando and kinetic results show that the active structure is the $\text{ZrO}_x\text{-Cu}$ boundary rather than Cu or ZrO_x alone. CO_2 first adsorbs on oxygen and hydroxyl sites in ZrO_x and forms carbonate or bicarbonate species. These species are then converted into bidentate formate. H_2 dissociates on nearby Cu sites, and surface hydrogen moves across the boundary. Formate is then converted into methoxy and methanol. Moderate ZrO_x coverage keeps CO_2 adsorption and hydrogenation sites close together. Excess ZrO_x separates stored intermediates from exposed Cu sites and slows further hydrogenation. During the 120 h test, the methanol rate decreased by only 6.8%. Post-reaction microscopy showed little change in Cu particle size, but the ZrO_x domains became partly aggregated. The loss of activity was therefore mainly related to a decrease in boundary length rather than Cu sintering. Earlier studies reported stable small ZrO_2 domains during shorter tests, but long-term changes in the oxide phase were not fully examined (Bao & Wang, 2026b; Mosayebi & Ahmadi, 2026). The present results show that stable ZrO_x dispersion is needed to maintain methanol production. However, only one reaction pressure and a limited range of Zr/Cu ratios were tested. Longer tests and direct measurements of boundary density are still needed.

4. Conclusion

ZrO_x modification improved CO_2 hydrogenation to methanol by forming active $\text{ZrO}_x\text{-Cu}$ interfaces. The catalyst with a Zr/Cu atomic ratio of 0.065 gave the best result. At 240 °C and 3.0 MPa, it reached a CO_2 conversion of 13.4%, a methanol selectivity of 71.9%, and a methanol space-time yield of 412.7 gMeOH kgcat⁻¹ h⁻¹. The apparent activation energy decreased from 86.5 to 58.2 kJ mol⁻¹, while the methanol formation rate increased by 3.6 times compared with unmodified Cu. Operando DRIFTS showed that bidentate formate formed at the $\text{ZrO}_x\text{-Cu}$ interface and was then converted into methoxy species. A kinetic isotope effect of 2.3 showed that hydrogen addition to formate was an important reaction step. During the 120 h test, the catalyst lost only 6.8% of its activity. This loss was mainly linked to partial ZrO_x aggregation rather than Cu sintering. This study links ZrO_x coverage with interface structure, formate hydrogenation, and catalyst stability under reaction conditions. The results may help develop Cu-based catalysts for low-temperature methanol production from CO_2 . However, only a limited range of Zr/Cu ratios and one reaction pressure were tested. Longer stability tests and direct measurements of interface density are still needed.

References

- [1].Baghdady, E. A., Medlin, J. W., & Schwartz, D. K. (2025). Tuning formate surface coverage with cosolvents for liquid-phase catalytic transfer hydrogenation. *Catalysis Science & Technology*, 15(11), 3354-3362.
- [2].Bao, Y., & Wang, H. (2026b). Edge-to-Cloud Infrastructure Continuum: A Unified Framework for Optimizing Industrial IoT Systems. Available at SSRN 7185578.
- [3].Bao, Y., Qiu, Y., & Wang, H. (2026a, May). Unified Identity Layer for Hyperscale Ecosystems: A Framework for Cross-Platform User Attribution and Experimentation. In 2026 6th International Conference on Machine Learning and Intelligent Systems Engineering (MLISE) (pp. 540-543). IEEE.
- [4].Chen, F., Liang, H., Li, S., Yue, L., & Xu, P. (2025). Design of Domestic Chip Scheduling Architecture for Smart Grid Based on Edge Collaboration.
- [5].Du, Y. (2025). Research on Digital Quality Traceability System for Temperature-Controlled Supply Chain of Foreign Trade Wine Driven by Blockchain and IoT. *Business and Social Sciences Proceedings*, 4, 57-65.
- [6].Goyal, A., Mondal, T., & Banerjee, A. (2026). Deciphering Binary and Ternary Interaction Effects in Inverse Cu – ZnO – ZrO₂ Catalysts for CO₂ Hydrogenation to Methanol. *The Journal of Physical Chemistry C*.
- [7].Gu, X. (2026). Identifying Causal Effects and Analyzing Heterogeneity of User Growth Interventions on Digital Platforms: Evidence from Large-Scale Behavioral Data. Available at SSRN 6809181.
- [8].Hadjiivanov, K., Panayotov, D., & Mihaylov, M. (2026). Isotopic labeling in IR spectroscopy of surface species: A powerful approach to advanced surface investigations. *Catalysts*, 16(1), 57.
- [9].Jiao, Y., Shi, T., Zhao, B., & Wang, A. (2026a). The Impact of VR Sketching Simulations on the Assessment of Scale and Site Suitability in Public Art Spaces.
- [10]. Jiao, Y., Zhao, B., Wang, A., & Shi, T. (2026b). Construction and Empirical Study of a Modularized Teaching System for Art Courses Based on a Unified Training Pathway.
- [11]. Kim, Y., Vu, M. P. U., Kim, H. J., & Park, H. (2026). First-principles calculations reveal precursor-dependent reaction mechanisms in ZrO₂ atomic layer deposition. *Scientific Reports*.
- [12]. Lee, M. K., Jeong, J. S., Jung, J., Seo, H. K., Shin, C., Kim, G. H., & Yang, M. K. (2026). Fast and energy-efficient resistive switching in ZrO_x/TaO_x bilayer structures under ultra-low voltage operation for next-generation memory applications. *Advanced Composites and Hybrid Materials*, 9(2), 143.
- [13]. Liang, R., Feifan, F. N. U., Liang, Y., & Ye, Z. (2025). Emotion-Aware Interface Adaptation in Mobile Applications Based on Color Psychology and Multimodal User State Recognition. *Frontiers in Artificial Intelligence Research*, 2(1), 51-57.
- [14]. Liang, S., Zhang, X., Du, Y., & Chen, W. (2026). Supply Network Restructuring and Capacity Ramp-Up Limits in the Localized Expansion of High-Performance Computing Equipment Production. Available at SSRN 7339738.

- [15]. Mohsen, A. A., & Allam, N. (2026). Bridging the Stability Gap in Perovskite Solar Cells: Mechanisms, Mitigation Strategies, and Commercial Perspectives. *Energy Advances*.
- [16]. Mosayebi, A., & Ahmadi, M. H. E. (2026). Enhanced syngas production via tri-reforming of methanol over promoted Ni/ZrO₂ catalysts: Influence of Cu, Co, and Ce on activity, stability, and carbon resistance. *International Journal of Hydrogen Energy*, 221, 154246.
- [17]. Moss, B., Liang, C., Carpenter, A., Verga, L. G., Scott, S., Jones, R. J., ... & Durrant, J. R. (2025). Operando ultraviolet – visible optical spectroelectrochemistry of surfaces. *Nature Reviews Methods Primers*, 5(1), 73.
- [18]. Phongprueksathat, N., Noh, G., Docherty, S. R., van Berkel, D. V., Stiefel, Y., Copéret, C., & Urakawa, A. (2026). Key Drivers of Activity and Selectivity in Cu - Based Catalysts for Methanol Synthesis From CO₂: Insights From Atomically Dispersed Promoters. *Angewandte Chemie International Edition*, e2693293.
- [19]. Todaro, S., Arena, F., Cannilla, C., Corrente, C., Cajumi, A., Samperi, M., ... & Bonura, G. (2026). Metal-oxide interfaces and oxygen vacancies as dominant active sites in CO₂ hydrogenation to methanol: contrasting reactivity of Cu-and In-based functionalities. *Applied Catalysis B: Environment and Energy*, 126614.
- [20]. Ughade, Y., Mehta, S., Patel, G., Gowda, R., Joshi, N., & Patel, R. (2025). Progress in CO₂ gas sensing technologies: Insights into metal oxide nanostructures and resistance-based methods. *Micromachines*, 16(4), 466.
- [21]. Wu, J., Wu, D., Zhang, J., & Peng, Y. (2026). Generative AI Feedback in Junior High School Artistic Creation Evaluation. Available at SSRN 7244838.
- [22]. Yang, J. (2026b). Stage - Coupled Computational Framework for Stratified Accessibility and Equity Analysis in Community - Based Elderly Care Services.
- [23]. Yang, Z., Alexandrova, A. N., & Sautet, P. (2026a). Modeling CO₂ Hydrogenation to Methanol on an Ensemble of Inverse ZrO₂ on Cu Catalytic Sites: Mechanism, Reactivity, and Deactivation. *Angewandte Chemie*, e5448247.
- [24]. You, S. (2026). Verifiable Audit Mechanisms in AI Compliance Automation: Scalability. Available at SSRN 6547458.