

MOF-Derived Cu–Ni–ZrO_x Interfaces for Efficient Hydrogenation of CO₂-Derived Intermediates

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Abstract

MOF-derived catalysts offer a controllable route to constructing highly dispersed metal–oxide interfaces for CO₂ conversion. Herein, HKUST-derived Cu–Ni–ZrO_x catalysts were synthesized by introducing Ni and Zr precursors during precursor reconstruction, followed by controlled calcination and reduction. The optimized Cu–Ni–ZrO_x catalyst achieved a CO₂ conversion of 16.8%, methanol selectivity of 81.5%, and methanol space–time yield of 538.6 gMeOH kgcat^{−1} h^{−1} at 250 °C and 3.0 MPa. Compared with Cu–ZrO_x, Ni incorporation increased the H₂ dissociation capacity by 44.7%, while ZrO_x stabilized formate and methoxy intermediates at the oxide–metal boundary. In situ DRIFTS showed faster conversion of formate to methoxy species, with the methoxy/formate intensity ratio increasing from 0.46 to 0.83 after Ni addition. The results indicate that MOF-derived Cu–Ni–ZrO_x catalysts improve methanol formation by coupling enhanced hydrogen activation with stabilized CO₂-derived intermediates.

Keywords: MOF-derived catalyst; Cu–Ni–ZrO_x; CO₂ hydrogenation; methanol; HKUST-1; interfacial catalyst; hydrogen activation

1. Introduction

CO₂ hydrogenation to methanol provides a promising route for the utilization of captured carbon and renewable hydrogen, while also contributing to chemical energy storage and the production of value-added fuels. Methanol is widely used as a chemical feedstock, liquid fuel, fuel additive, and hydrogen carrier, making its synthesis from CO₂ attractive from both environmental and industrial perspectives. However, the high thermodynamic stability of CO₂ and the multiple hydrogen-transfer steps required for C–O bond transformation make selective methanol formation kinetically difficult. The reverse water–gas shift (RWGS) reaction competes strongly with methanol synthesis, particularly at elevated temperatures, where CO formation becomes increasingly favorable. Cu-based catalysts are widely investigated because metallic Cu efficiently activates H₂ and supports the hydrogenation of carbon-containing intermediates under relatively moderate conditions. Their catalytic behavior, however, is strongly affected by Cu particle size, oxidation state, local coordination environment, and interaction with neighboring oxide phases

[1,2]. Increasing evidence indicates that Cu–oxide interfacial sites play a central role in CO₂ activation and subsequent hydrogenation. Metallic Cu mainly supplies dissociated hydrogen, whereas Cu⁺ species, oxygen defects, hydroxyl groups, and coordinatively unsaturated oxide sites assist the adsorption and stabilization of CO₂-derived intermediates [3,4]. Recent theoretical analysis of inverse ZrO₂/Cu catalysts further showed that the active interface should be viewed as an ensemble of structurally different catalytic configurations instead of a single static site. Only a fraction of the accessible interfacial structures remained highly active throughout the complete methanol pathway, while the catalytic rate was strongly affected by steps occurring after methoxy formation. Structural evolution from more active configurations toward less active states was also proposed as an important origin of activity loss [5]. These findings emphasize that both interfacial composition and structural stability under reaction conditions must be considered when designing Cu-based methanol catalysts.

ZrO₂ is particularly attractive as an oxide component because it contains adjustable acid–base sites, surface hydroxyl groups, and oxygen-deficient sites that can promote CO₂ adsorption and stabilize bicarbonate, carbonate, formate, and methoxy species. When Cu and ZrO₂ are brought into close contact, CO₂-derived species can be adsorbed on Zr-containing sites while hydrogen supplied by neighboring Cu sites participates in their sequential hydrogenation. Studies of conventional Cu/ZrO₂ and inverse ZrO₂/Cu catalysts have consistently shown that the metal–oxide boundary contributes strongly to CO₂ activation and methanol formation [6,7]. The inverse configuration is especially interesting because highly dispersed ZrO_x species on Cu can generate a large number of perimeter sites with short distances between CO₂ adsorption centers and hydrogen-dissociation sites. Such proximity can facilitate hydrogen transfer toward adsorbed formate and methoxy intermediates. At the same time, the amount and distribution of ZrO_x must be carefully controlled. Excessive oxide coverage can block accessible Cu surface sites and decrease the number of locations available for H₂ dissociation, whereas insufficient Cu–ZrO_x contact can restrict interfacial hydrogen transfer. Strong stabilization of carbonate or formate species may also produce inactive surface reservoirs when their further hydrogenation becomes slower than their formation. The optimum catalyst therefore requires a balance among CO₂ adsorption strength, hydrogen availability, intermediate mobility, and the density of accessible Cu–ZrO_x boundaries. Introducing a second metallic component offers another route to regulate this balance. Ni is able to dissociate H₂ efficiently and can increase the concentration of reactive surface hydrogen available for hydrogenation reactions. When appropriately incorporated into a Cu-containing catalyst, Ni may accelerate hydrogen transfer toward adsorbed formate, methoxy, and related oxygenated intermediates and thereby improve the utilization of CO₂-derived surface species [8,9]. Its promotional effect is nevertheless highly dependent on composition and local structure. A low or moderate Ni content may improve H₂ activation without substantially changing the product distribution, whereas excessive Ni loading, large Ni-rich particles, or unsuitable Cu–Ni interactions can promote deeper hydrogenation or alter the preferred reaction pathway. These

changes may increase CO or CH₄ formation and consequently decrease methanol selectivity [10,11]. Cu–Ni alloying can also modify the electronic structure of surface Cu atoms and change the adsorption strength of hydrogen and carbon-containing intermediates. The catalytic function of Ni therefore cannot be evaluated only from its total loading. Its particle size, dispersion, alloying degree, oxidation state, and spatial relationship with both Cu and ZrO_x must be considered. A carefully constructed Cu–Ni–ZrO_x interface could provide complementary catalytic functions in which Cu favors methanol-forming hydrogenation chemistry, Ni increases the supply of activated hydrogen, and ZrO_x provides adsorption and stabilization sites for CO₂-derived oxygenates. Effective cooperation among these functions requires short transport distances and intimate contact among the three components. Achieving such nanoscale contact by conventional impregnation or sequential deposition can be difficult because different precursors may undergo independent nucleation, migration, agglomeration, and phase separation during calcination and reduction. Metal–organic frameworks (MOFs) provide an alternative precursor platform for controlling the spatial distribution of multiple catalytic components. Their porous architectures, high metal dispersion, and structurally defined coordination environments allow different elements to be introduced and mixed before thermal transformation. During calcination and reduction, the organic framework can be removed while the preorganized metal species are converted into metallic particles and oxide domains with relatively short intercomponent distances. MOF-derived Cu–Zn and Cu–Ce catalysts have demonstrated that this strategy can generate smaller particles, more uniform elemental distributions, and increased metal–oxide interfacial contact compared with many conventionally prepared catalysts [12,13]. These structural characteristics are particularly relevant to CO₂ hydrogenation because catalytic performance depends strongly on the probability that adsorbed CO₂-derived intermediates encounter nearby activated hydrogen. HKUST-type materials are attractive Cu-containing precursors because Cu is already incorporated into the framework at the molecular level, providing a basis for introducing additional promoters during precursor modification or reconstruction. Incorporation of Ni and Zr species before thermal treatment may therefore create a more integrated Cu–Ni–Zr distribution than post-synthetic deposition onto preformed Cu particles. Despite this potential, most MOF-derived catalysts reported for CO₂-to-methanol conversion have concentrated on Cu–Zn or related binary systems [14,15]. The formation, structural evolution, and catalytic behavior of HKUST-derived Cu–Ni–ZrO_x interfaces remain much less understood. Another limitation in the current literature is the difficulty of establishing a direct relationship between catalyst structure, surface intermediates, and methanol productivity. Many studies examine only a limited number of compositions, making it difficult to distinguish genuine promotional effects from changes caused by metal loading, particle size, or exposed surface area. Reaction conditions also vary widely in pressure, temperature, H₂/CO₂ ratio, gas hourly space velocity, catalyst mass, and product calculation method, which limits direct comparison among reported catalysts. Short-duration catalytic tests may further overlook structural reconstruction, sintering, oxide migration, or

changes in metal oxidation state occurring during extended operation. Ex situ X-ray diffraction, X-ray photoelectron spectroscopy, and electron microscopy provide valuable information on bulk phases, particle morphology, and surface composition before or after reaction, but they cannot fully describe the dynamic catalyst surface during CO₂ hydrogenation. This issue is important for Cu–oxide systems because oxidation state, hydroxyl coverage, interfacial structure, and adsorbate population can respond continuously to the surrounding H₂/CO₂/H₂O atmosphere. In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) can follow bicarbonate, carbonate, formate, methoxy, and other adsorbed species under reaction-relevant conditions and is therefore useful for studying reaction pathways [16,17]. However, the observation of a strong infrared band alone cannot establish that the corresponding species is a kinetically relevant intermediate. A highly populated formate species, for instance, may represent either a productive intermediate or a relatively stable spectator accumulated on the oxide surface. Mechanistic interpretation becomes more reliable when the evolution of formate and methoxy species is correlated with H₂ activation, catalyst composition, methanol formation rate, and product selectivity under comparable conditions [18]. Such an integrated approach is particularly necessary for ternary Cu–Ni–ZrO_x catalysts, where changing Ni or Zr content can simultaneously influence H₂ dissociation, CO₂ adsorption, intermediate stability, metal dispersion, and the number of accessible interfacial sites.

Against this background, the present study develops HKUST-derived Cu–Ni–ZrO_x catalysts in which Ni and Zr precursors are introduced during precursor reconstruction, followed by controlled calcination and reduction to generate closely contacted metallic and oxide domains. The central objective is to determine how the balance between H₂ activation and stabilization of CO₂-derived intermediates governs methanol formation over this ternary interface. Particular attention is given to whether an appropriate amount of Ni can increase H₂ dissociation and the availability of reactive hydrogen without driving the reaction toward excessive CO or CH₄ formation, and whether dispersed ZrO_x can provide suitable adsorption environments for formate and methoxy species while maintaining sufficient exposure of Cu-containing hydrogenation sites. Catalyst composition, crystalline structure, particle morphology, elemental distribution, surface chemical state, and metal–oxide interaction are examined together with hydrogen uptake behavior to establish how precursor composition controls the resulting catalytic interface. CO₂ conversion, methanol selectivity, by-product distribution, and methanol space–time yield are evaluated under consistent reaction conditions so that changes in catalytic performance can be directly related to structural and surface properties. In situ DRIFTS is further employed to monitor the evolution of adsorbed CO₂-derived species, with emphasis on the formation and subsequent transformation of formate and methoxy intermediates. Correlating these spectroscopic observations with hydrogen uptake and methanol productivity provides a basis for distinguishing productive intermediate conversion from simple surface accumulation. Through this combined structural, kinetic, and spectroscopic analysis, the study seeks to clarify how Ni-assisted H₂ activation and ZrO_x-mediated intermediate stabilization can be coordinated at Cu-based interfaces. The results are expected to

provide a mechanistic basis for controlling the composition and spatial organization of multifunctional Cu–Ni–oxide catalysts and to demonstrate how MOF-derived precursors can be used to construct closely coupled catalytic sites for selective CO₂ hydrogenation to methanol.

2. Materials and Methods

2.1. Catalyst Samples and Reaction Conditions

Six catalysts were prepared, including HKUST-derived Cu, Cu–ZrO_x, Cu–Ni, and three Cu–Ni–ZrO_x samples with different Ni contents. The nominal Ni contents were 1, 3, and 5 wt%, while the Zr content was fixed at 8 wt%. HKUST-1 was prepared from copper nitrate and trimesic acid in an ethanol–water solution. Ni and Zr precursors were added during precursor reconstruction to improve their contact with the Cu phase. The solids were washed, dried at 80 °C, calcined in air at 350 °C, and reduced in H₂ at 300 °C. CO₂ hydrogenation was carried out in a stainless-steel fixed-bed reactor at 220–280 °C and 3.0 MPa. The H₂/CO₂ molar ratio was 3:1, and N₂ was used as an internal standard. The total gas flow rate was 80 mL min^{−1}, and 200 mg of catalyst was used in each test. Each condition was repeated three times.

2.2. Experimental Design and Control Tests

The catalyst groups were used to separate the roles of Cu, Ni, and ZrO_x in methanol formation. HKUST-derived Cu served as the base catalyst. Cu–ZrO_x was used to study the effect of oxide sites on CO₂ adsorption and intermediate binding. Cu–Ni was used to examine the effect of Ni on H₂ dissociation without ZrO_x. The three Cu–Ni–ZrO_x samples were compared to identify a suitable Ni content for faster hydrogen transfer without a clear increase in CO or CH₄ formation. A physical mixture of Cu–Ni and ZrO₂ was also tested. Its overall composition was the same as that of the best Cu–Ni–ZrO_x catalyst. This control was used to distinguish close interface contact from simple particle mixing. Blank tests were conducted without a catalyst and under H₂/N₂ without CO₂. Before each activity test, the catalyst was reduced in 10 vol% H₂/N₂ at 300 °C for 2 h. The reaction was kept at each temperature for 3 h before gas samples were collected.

2.3. Characterization and Quality Control

Crystal phases were identified by X-ray diffraction using Cu K α radiation. Particle size, pore structure, and element distribution were examined by transmission electron microscopy, high-angle annular dark-field imaging, and energy-dispersive X-ray mapping. The surface states of Cu, Ni, Zr, and O were measured by X-ray photoelectron spectroscopy. The C 1s peak at 284.8 eV was used for binding-energy correction. Surface area and pore volume were measured by N₂ adsorption at −196 °C. H₂ chemisorption and H₂ temperature-programmed desorption were used to compare hydrogen uptake and H₂ activation. Surface formate and methoxy species were measured by in situ diffuse reflectance infrared Fourier-transform spectroscopy under CO₂/H₂ flow. Reaction products were analysed by online gas chromatography. Methanol and other

oxygenates were measured with a flame-ionization detector. CO₂, CO, H₂, and N₂ were measured with a thermal-conductivity detector. Calibration curves were prepared using certified gas mixtures and liquid standards. Data were accepted when the carbon balance was between 95% and 105% and the difference among repeated tests was below 5%.

2.4. Data Processing and Performance Calculations

Gas concentrations were corrected using the N₂ internal standard. CO₂ 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 CO₂, respectively.

Methanol selectivity was calculated on a carbon basis as

$$S_{\text{MeOH}}(\%) = \frac{F_{\text{MeOH},\text{out}}}{F_{\text{MeOH},\text{out}} + F_{\text{CO},\text{out}} + F_{\text{CH}_4,\text{out}}} \times 100,$$

where $F_{\text{MeOH},\text{out}}$, $F_{\text{CO},\text{out}}$, and $F_{\text{CH}_4,\text{out}}$ are the outlet molar flow rates of methanol, CO, and CH₄, respectively. The methanol space–time yield was calculated from the methanol production rate per unit catalyst mass. The methoxy/formate intensity ratio was obtained from the integrated DRIFTS band areas after baseline correction. Results were reported as mean values with standard deviations. Differences among the catalyst groups were tested by one-way analysis of variance followed by Tukey’s test. A value of $p < 0.05$ was considered significant.

2.5. In Situ Intermediate Analysis and Stability Tests

In situ DRIFTS was used to monitor carbonate, bicarbonate, formate, methoxy, and adsorbed CO species during CO₂ hydrogenation. Each catalyst was first reduced in H₂ and then exposed to the CO₂/H₂ feed at 250 °C and 3.0 MPa. Spectra were collected every 2 min until the band intensities became stable. Step-response tests were then conducted by switching from CO₂/H₂ to H₂ alone. The decrease in formate bands and the increase in methoxy bands were used to compare the hydrogenation rates of surface intermediates. Catalyst stability was tested at 250 °C and 3.0 MPa for 50 h. After the test, XRD, TEM, XPS, and N₂ adsorption measurements were repeated to examine particle growth, Cu and Ni oxidation, pore loss, and ZrO_x movement. The catalyst was considered stable when the methanol space–time yield decreased by less than 10% and no clear phase change was observed.

3. Results and Discussion

3.1. Precursor Conversion and H₂ Activation

XRD and electron microscopy showed that the HKUST precursor formed a porous Cu-based catalyst after calcination and reduction. Cu, Ni, and Zr were evenly distributed in the optimized sample. No large Ni or ZrO_x particles were detected. This structure created close contact among

Cu, Ni, and ZrO_x while leaving part of the Cu surface exposed. XPS showed shifts in the Cu and Ni binding energies after the three components were combined. These shifts indicate electron transfer at the interface. H_2 chemisorption and temperature-programmed desorption showed that Ni addition increased the H_2 dissociation capacity by 44.7% compared with Cu- ZrO_x , as shown in Fig. 1. A moderate Ni content gave the largest increase. Further Ni addition produced Ni-rich regions, covered part of the Cu surface, and increased strong hydrogen adsorption. Atta et al. (2025) reported that MOF-5 improved metal dispersion and methanol production in Cu/ZnO/CeO₂ catalysts. Burwell et al. (2026) also found that a UiO-67-derived ZrO_2 structure limited Cu particle growth and formed more Cu- ZrO_2 interface sites. The present catalyst adds Ni to this structure to improve H_2 activation.

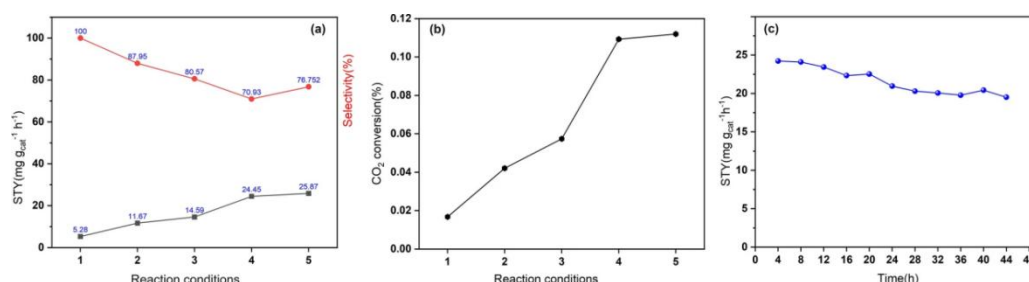


Fig. 1. Structure, H_2 adsorption, and CO_2 hydrogenation performance of HKUST-derived Cu catalysts.

3.2. Effect of Catalyst Composition on Methanol Production

Catalytic performance depended on the contact among Cu, Ni, and ZrO_x . Cu- ZrO_x showed high methanol selectivity but lower CO_2 conversion because its H_2 activation capacity was limited. Cu-Ni improved CO_2 conversion, but the absence of ZrO_x reduced the number of sites for binding formate and methoxy species. The Cu-Ni- ZrO_x catalysts combined the two effects. The optimized sample reached a CO_2 conversion of 16.8%, a methanol selectivity of 81.5%, and a methanol space-time yield of 538.6 gMeOH kgcat⁻¹ h⁻¹ at 250 °C and 3.0 MPa, as shown in Fig. 1. Methanol production first increased with Ni content and then decreased at the highest loading. Moderate Ni addition supplied more active hydrogen. Excess Ni increased CO formation and covered part of the Cu- ZrO_x interface. The physical mixture gave a lower methanol yield than the MOF-derived catalyst with the same overall composition. This result shows that close interface contact was more important than composition alone [19,20]. Hoang et al. (2025) reported a methanol selectivity of 79% over a MOF-5-based Cu/ZnO/CeO₂ catalyst. Satheesh et al. (2026) found that a MOF-derived Cu- ZrO_2 catalyst produced more methanol than a catalyst prepared by a common method. However, direct comparison remains difficult because the reaction pressure, flow rate, catalyst mass, and yield units differed among studies.

3.3. Conversion of Formate into Methoxy Species

In situ DRIFTS detected carbonate, bicarbonate, formate, and methoxy species during CO₂ hydrogenation. Formate was the main surface carbon species on Cu–ZrO_x. Its slow decrease under H₂ showed that further hydrogenation was limited. Ni addition changed this behaviour. The formate bands decreased faster, while the methoxy bands increased. The methoxy/formate intensity ratio increased from 0.46 on Cu–ZrO_x to 0.83 on the optimized Cu–Ni–ZrO_x catalyst, as shown in Fig. 2. This result agrees with the higher H₂ dissociation capacity after Ni addition [21,22]. H₂ was dissociated on Cu and Ni sites, and the surface hydrogen then moved to formate species near ZrO_x. ZrO_x helped adsorb CO₂ and kept formate and methoxy species close to the metal sites. Bao et al. (2026) found that the loss of ZrO₂-bound formate was related to the formation of methoxy species on Cu/ZrO₂. Their results also showed that formate hydrogenation was a slow step. Nimmas et al. (2026) reported that Ni promoted the hydrogenation of formate and methoxy species. The present results show that Ni-assisted H₂ activation and ZrO_x-assisted intermediate binding can occur in the same MOF-derived catalyst.

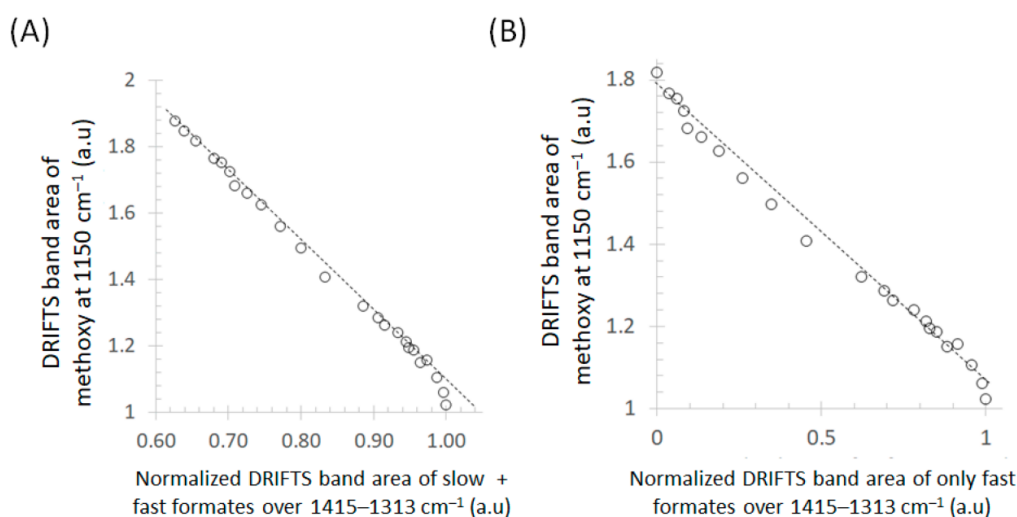


Fig. 2. Formate and methoxy species and the methanol formation route at Cu–Ni–ZrO_x interfaces.

3.4. Interface Reaction Route and Catalyst Stability

The results suggest that Cu, Ni, and ZrO_x have different roles during methanol formation. CO₂ first adsorbed on oxygen and hydroxyl sites near ZrO_x and formed carbonate or bicarbonate species. These species were then hydrogenated to formate. Cu and Ni dissociated H₂, while Ni increased the amount of active surface hydrogen. The hydrogen moved to the oxide–metal interface and converted formate into methoxy species. Methoxy was then hydrogenated to methanol. Faster formate-to-methoxy conversion explains the higher methanol yield after Ni addition. The Cu–Ni–ZrO_x interface also reduced direct CO formation by keeping CO₂-derived species near the hydrogenation sites. Post-reaction tests showed only small changes in particle distribution and surface state after 50 h. Wu et al. (2026) also reported stable methanol production over a MOF-derived Cu–ZrO₂ catalyst during a 100 h test. However, the present study tested only a limited range of Ni and Zr contents, one reaction pressure, and a 50 h period. DRIFTS also

provides average surface signals and cannot identify the exact location of each active species [23,24]. Further studies should use operando X-ray absorption, isotope-switching tests, and longer stability runs under different H₂/CO₂ ratios.

4. Conclusion

The HKUST-derived Cu–Ni–ZrO_x catalyst improved CO₂ hydrogenation to methanol through the combined effects of Cu, Ni, and ZrO_x. The best sample reached a CO₂ conversion of 16.8%, a methanol selectivity of 81.5%, and a methanol space–time yield of 538.6 gMeOH kgcat^{−1} h^{−1} at 250 °C and 3.0 MPa. Ni increased H₂ dissociation by 44.7%, while ZrO_x helped retain formate and methoxy species near the metal–oxide interface. In situ DRIFTS showed faster conversion of formate into methoxy after Ni addition. The methoxy/formate intensity ratio increased from 0.46 to 0.83. These results show that methanol production depends on both H₂ activation and the further hydrogenation of CO₂-derived species. The main feature of this study is the use of an HKUST-based method to form close contact among Cu, Ni, and ZrO_x. This structure links H₂ activation with intermediate conversion. The catalyst may be useful for CO₂-based methanol production. However, only a narrow range of metal contents, one pressure, and a 50 h stability period were tested. Further studies should examine more catalyst compositions, longer reaction times, different feed ratios, and operando tests under reaction conditions.

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