



Alkali-Regulated Acid–Base Balance for Selective C1 Oxygenate Production over Oxide-Modified Copper Catalysts

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ABSTRACT

The selective hydrogenation of CO₂ into oxygenated C1 products requires a balanced distribution of basic CO₂ adsorption sites, hydrogen activation sites, and interfacial hydrogenation centers. In this work, alkali-assisted regulation of oxide-modified copper catalysts was investigated to clarify how surface acid–base properties influence methanol selectivity. A series of Na-, K-, and Cs-promoted Cu–ZrOx catalysts were synthesized by sequential impregnation, with alkali loadings ranging from 0.2 to 2.0 wt%. Catalytic performance was evaluated at 230–270 °C, 3.0 MPa, and H₂/CO₂ = 3. The 0.8 wt% K-promoted catalyst showed the best performance, achieving a CO₂ conversion of 14.7%, methanol selectivity of 78.3%, and methanol space–time yield of 468.5 gMeOH kgcat^{−1} h^{−1} at 250 °C. Compared with the unpromoted catalyst, the CO selectivity decreased from 28.6% to 15.9%, while the apparent activation energy for methanol formation decreased from 72.8 to 57.6 kJ mol^{−1}. CO₂-TPD results showed that moderate K addition increased the density of medium-strength basic sites from 186 to 312 μmol gcat^{−1}, enhancing CO₂ adsorption without causing excessive carbonate accumulation. In situ DRIFTS revealed that K promotion strengthened the formation of reactive formate species at 1582 and 1365 cm^{−1}, while suppressing linearly adsorbed CO on Cu sites. However, alkali loadings above 1.5 wt% reduced methanol productivity by blocking Cu surface sites required for H₂ dissociation. Kinetic analysis indicated that the optimized catalyst exhibited a CO₂ reaction order of 0.38 and an H₂ reaction order of 0.94, suggesting that hydrogen supply remained kinetically important after alkali modification. These results demonstrate that alkali promoters improve methanol selectivity mainly by tuning the acid–base balance at oxide–copper interfaces rather than simply increasing CO₂ uptake. This study provides a practical strategy for improving C1 oxygenate formation through controlled surface basicity.

1. Introduction

CO₂ hydrogenation to methanol has attracted considerable attention as a route for carbon utilization and renewable hydrogen storage. Methanol is not only an important bulk chemical and fuel but also a convenient liquid hydrogen carrier and a versatile intermediate for the production of olefins, aromatics, and other value-added chemicals. Its synthesis from CO₂ and H₂ therefore provides a potential link between carbon recycling and hydrogen-based energy systems. Cu-based catalysts remain among the most widely investigated materials for this reaction because metallic and partially oxidized Cu species can facilitate H₂ activation and promote the sequential hydrogenation of carbon-containing intermediates under relatively moderate reaction conditions. However, Cu

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alone interacts only weakly with CO₂ and generally provides an insufficient number of sites for efficient CO₂ adsorption and activation. The catalytic behavior is therefore strongly influenced by the oxide component and, in particular, by the nature of the metal–oxide interface. Studies on Cu catalysts combined with ZnO, ZrO₂, CeO₂, and TiO₂ have shown that methanol productivity depends not simply on Cu loading or total surface area, but also on Cu particle size, oxide composition, surface coordination, defect density, and the extent of metal–oxide contact (Chen et al., 2025; Esmaili et al., 2026). Recent theoretical analysis further demonstrated that inverse ZrO₂/Cu interfaces contain an ensemble of structurally distinct catalytic configurations rather than a single uniform active site. Only a fraction of the accessible configurations remain highly active throughout the complete CO₂-to-methanol pathway, while the stability of methoxy-containing structures and reaction steps occurring after methoxy formation can substantially influence the overall turnover rate and catalyst deactivation behavior (Yang et al., 2026). These findings reinforce the view that the Cu–oxide boundary is a dynamically heterogeneous reaction environment whose local structure controls both intermediate stabilization and catalytic performance. Related experimental studies have likewise connected methanol formation with Cu–oxide interfacial structure, oxygen vacancies, and surface electronic states (Liang et al., 2025).

Among the oxide components used with Cu, ZrO₂ is particularly attractive because of its adjustable acid–base properties, thermal stability, oxygen-vacancy chemistry, and ability to provide adsorption sites for oxygen-containing intermediates. ZrO₂ can enhance CO₂ adsorption through surface hydroxyl groups, basic oxygen atoms, and defect-associated sites, while adjacent Cu species supply activated hydrogen for subsequent hydrogenation. The close spatial coupling of these functions is important because efficient methanol formation requires not only CO₂ adsorption but also rapid hydrogen transfer across the Cu–ZrO₂ boundary. Surface formate is generally regarded as an important intermediate in this pathway, although its catalytic role is more complex than its spectroscopic abundance alone may suggest. Infrared studies of Cu/ZrO₂ have revealed the simultaneous formation of several formate species with different coordination environments and reactivities. Some formate species can be hydrogenated relatively rapidly toward methoxy and methanol, whereas others accumulate on the surface and behave mainly as slowly reacting spectators (Haider et al., n.d.). Consequently, a strong formate signal does not necessarily indicate a high methanol formation rate. Changes in ZrO₂ defect density and Cu–ZrO₂ contact can modify the relative stability of formate, methoxy, carbonate, and adsorbed CO species and thereby alter competition between methanol synthesis and the reverse water–gas shift pathway (Du, 2025; Todaro et al., 2026). The geometric arrangement of Cu and Zr-containing sites, as well as the availability of oxygen vacancies, can additionally influence hydrogen spillover and the local electronic environment of adsorbed intermediates (Jiao et al., 2026a). These observations indicate that the catalytic function of ZrO₂ is determined by the distribution and strength of individual surface sites rather than by oxide content alone. Surface promotion provides a practical strategy for further tuning this interfacial chemistry. Alkali metals such as Na, K, and Cs can substantially modify the acid–base and electronic properties of Cu-based catalysts even at relatively low loadings. Their introduction generally increases surface basicity and may strengthen interactions between CO₂-derived species and the catalyst surface. At the same time, alkali cations can redistribute charge near Cu and oxide atoms, influence oxygen-vacancy environments, and alter the adsorption geometry and stability of carbonate, bicarbonate, formate, methoxy, and CO species. The resulting effect on methanol synthesis is therefore more complex than a simple increase in total CO₂ adsorption. Previous studies have shown that catalytic performance depends strongly on promoter identity, concentration, and spatial location (Yang, 2026). In particular, appropriately positioned Na⁺ species near isolated or interfacial Cu sites have been associated with improved site stability

and enhanced methanol selectivity, whereas K^+ and Cs^+ can generate different electronic and steric effects because of their larger ionic sizes and different interaction strengths with the support (Bagchi et al., 2026). Related investigations of $CuZn-CeO_x$ and $CuZn/ZnZrO_x$ systems have further linked methanol formation to promoter-induced changes in local charge distribution, vacancy populations, hydrogen-transfer behavior, and stabilization of oxygenated intermediates (Kumar & Srivastava, 2026). These results suggest that alkali promotion can affect several elementary processes simultaneously, including CO_2 capture, H_2 activation, intermediate hydrogenation, CO desorption, and surface-site regeneration. The beneficial effect of increasing basicity nevertheless has clear limits. Excessive alkali loading can partially cover exposed Cu sites, reduce the number of ensembles available for H_2 dissociation, or alter $Cu-ZrO_2$ contact in an unfavorable manner. Strongly basic surfaces may also stabilize carbonate or bicarbonate species to such an extent that these species become kinetically difficult to hydrogenate. Under such conditions, high CO_2 uptake can coexist with low catalytic turnover (Wu et al., 2026). Similar non-monotonic relationships between promoter loading, basicity, and methanol productivity have been reported for other alkali-modified Cu systems. This distinction is particularly important for interpreting CO_2 temperature-programmed desorption measurements (Engel et al., 2025; Gu, 2026). Total desorption capacity alone does not distinguish weak sites that release CO_2 readily from medium-strength sites capable of stabilizing reactive intermediates or from strong sites that may retain carbon-containing species excessively. A catalyst with the highest total basicity is therefore not necessarily the most effective catalyst for methanol synthesis. The relative populations of weak, medium, and strong basic sites may provide a more informative description of the surface environment. At the same time, spectroscopic identification of formate or adsorbed CO cannot by itself establish whether these species participate directly in the productive catalytic cycle. Surface intermediates detected under reaction conditions may represent rapidly converting species, kinetically relevant resting states, or comparatively inert spectator species. Their contribution must therefore be evaluated together with catalytic rates and kinetic parameters (Bao et al., 2026; Boorla & Maranas, 2025). Despite substantial progress in understanding Cu -based methanol catalysts, a systematic relationship between alkali identity, promoter loading, basic-site distribution, surface intermediates, and reaction kinetics remains insufficiently established for $Cu-ZrO_x$ systems. Direct comparisons of Na -, K -, and Cs -promoted $Cu-ZrO_x$ catalysts prepared and evaluated under identical conditions are still limited, making it difficult to separate intrinsic promoter effects from differences in catalyst preparation, Cu dispersion, support structure, and reaction protocol. Moreover, many studies characterize alkali promotion mainly through total CO_2 adsorption or overall basicity, without resolving how the distribution of weak, medium-strength, and strong basic sites changes with promoter loading. This limitation makes it difficult to determine which type of basic site is most closely associated with productive CO_2 activation. A similar uncertainty exists in the interpretation of surface intermediates because higher formate coverage does not necessarily correspond to faster formate conversion or higher methanol productivity (Jiao et al., 2026b; You, 2026). Establishing a direct connection between surface acid-base properties, intermediate evolution, and kinetic behavior is therefore necessary to clarify how alkali promoters regulate the $Cu-ZrO_x$ interface. In the present study, Na -, K -, and Cs -promoted $Cu-ZrO_x$ catalysts with alkali loadings ranging from 0.2 to 2.0 wt% were systematically investigated to determine how promoter identity and concentration regulate CO_2 hydrogenation to methanol. Rather than correlating catalytic activity solely with total alkali content or total CO_2 adsorption, the study focuses on the distribution of basic-site strengths and its relationship with the availability of Cu sites and the evolution of surface intermediates. CO_2 -TPD was employed to distinguish changes in weak, medium-strength, and strong basic sites, while in situ DRIFTS was used to follow the formation and transformation of

formate and adsorbed CO species under reaction-relevant conditions. Catalytic measurements were further combined with apparent activation energies and reaction orders with respect to CO₂ and H₂ to provide kinetic evidence for promoter-induced changes in the reaction pathway. Through this integrated analysis, the work aims to identify an alkali-loading regime that increases the population of catalytically useful medium-strength basic sites while avoiding excessive stabilization of carbonate-derived species and blockage of Cu sites required for H₂ activation. Comparison among Na, K, and Cs additionally provides a basis for distinguishing the effects of alkali concentration from those arising from promoter-specific electronic and steric properties. The broader significance of this study is to establish a mechanistic relationship between alkali-controlled surface acid–base balance, Cu–ZrO_x interfacial chemistry, intermediate reactivity, and product selectivity. Such understanding can explain why enhanced CO₂ adsorption does not necessarily translate into higher methanol productivity and can provide a more rational basis for designing promoted Cu–ZrO_x catalysts that simultaneously favor methanol formation, suppress CO production, and maintain effective hydrogen activation.

2. Materials and Methods

2.1 Catalyst Samples and Feed Gases

Nineteen Cu–ZrO_x catalysts were prepared. One unpromoted Cu–ZrO_x sample was used as the reference catalyst. The other 18 samples were modified with Na, K, or Cs at loadings of 0.2, 0.5, 0.8, 1.0, 1.5, and 2.0 wt%. Cu–ZrO_x was prepared by co-precipitation from copper nitrate and zirconyl nitrate solutions at 65 °C and pH 9.0. The precipitate was aged for 4 h, filtered, washed with deionized water, dried at 110 °C for 12 h, and calcined at 450 °C for 4 h. Na, K, and Cs were then added by pore-volume impregnation using the corresponding nitrate solutions. The promoted samples were dried at 110 °C and calcined at 400 °C for 3 h. Before testing, all catalysts were sieved to 250–425 µm. CO₂, H₂, N₂, He, and Ar with purities above 99.999% were used.

2.2 Reaction Design and Control Tests

CO₂ hydrogenation was carried out in a stainless-steel fixed-bed reactor with an inner diameter of 8 mm. Each test used 0.30 g of catalyst mixed with 0.60 g of quartz particles. Before reaction, the catalyst was reduced in 20 vol% H₂/N₂ at 300 °C for 3 h. The reaction temperature ranged from 230 to 270 °C, and the total pressure was 3.0 MPa. The H₂/CO₂ molar ratio was fixed at 3, and the gas hourly space velocity was 12,000 mL g_{cat}^{−1} h^{−1}. Unpromoted Cu–ZrO_x was used as the main control. Samples with the same alkali loading were compared to study the effect of alkali type. Samples with different loadings of the same alkali were used to study the effect of promoter amount. Blank tests with quartz and bare ZrO_x produced no measurable methanol. The catalyst containing 0.8 wt% K was tested for 100 h at 250 °C to measure long-term stability.

2.3 Characterization and Quality Control

Crystal phases were identified by X-ray diffraction with Cu Kα radiation. Surface area and pore volume were measured by N₂ adsorption at −196 °C. Cu, Zr, and alkali contents were measured by inductively coupled plasma optical emission spectroscopy. Particle size and element distribution were examined by transmission electron microscopy and high-angle annular dark-field scanning transmission electron microscopy. Surface oxidation states were measured by X-ray photoelectron spectroscopy. CO₂ temperature-programmed desorption was used to measure the amount and strength of basic sites. H₂ chemisorption was used to estimate the number of exposed Cu sites. H₂ temperature-programmed reduction was used to study catalyst reduction. In situ DRIFTS spectra were collected from 1000 to 2200 cm^{−1} under CO₂/H₂ flow at 250 °C. Reaction products were measured by online gas chromatography with thermal-conductivity and flame-ionization detectors. Gas flow meters were calibrated before each test series. Carbon balances were kept between 97%

and 103%. Each catalytic test was repeated three times. Tests with a relative error above 5% were repeated.

2.4 Data Processing and Model Equations

CO₂ conversion was calculated from the inlet and outlet molar flow rates:

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

where $F_{\text{CO}_2,\text{in}}$ and $F_{\text{CO}_2,\text{out}}$ are the inlet and outlet CO₂ molar flow rates, respectively. Methanol selectivity was calculated on a carbon basis:

$$S_{\text{CH}_3\text{OH}} = \frac{F_{\text{CH}_3\text{OH}}}{F_{\text{CH}_3\text{OH}} + F_{\text{CO}} + F_{\text{CH}_4}} \times 100\%$$

where $F_{\text{CH}_3\text{OH}}$, F_{CO} , and F_{CH_4} are the outlet molar flow rates of methanol, CO, and methane. Methanol space–time yield was calculated from the methanol flow rate and catalyst mass. CO₂-TPD peaks were grouped into weak, medium, and strong basic-site regions according to desorption temperature. DRIFTS spectra were corrected for baseline changes and normalized by catalyst mass. The peak areas at 1582 and 1365 cm⁻¹ were used to compare formate species among the catalysts.

2.5 Kinetic and Statistical Analysis

Kinetic measurements were started after the outlet composition remained stable for at least 2 h. Apparent activation energies were calculated from reaction rates measured between 230 and 260 °C. CO₂ conversion was kept below 10% to limit heat- and mass-transfer effects. Reaction orders were measured by changing the partial pressure of CO₂ or H₂ while keeping the total pressure and flow rate constant. External mass transfer was checked by changing the total gas flow from 60 to 140 mL min⁻¹. Internal diffusion was tested with catalyst particle sizes of 150–250, 250–425, and 425–600 μm. No clear rate difference was found between the two smaller particle ranges. Pearson correlation analysis was used to compare methanol yield with medium-strength basic-site density, exposed Cu area, formate peak area, and CO coverage. Differences among catalysts were tested by one-way analysis of variance followed by Tukey's test. Differences were considered significant at $p < 0.05$. Results are reported as the mean ± standard deviation of three independent tests.

3. Results and Discussion

3.1 Effect of Alkali Type and Loading on Catalytic Performance

Alkali addition changed CO₂ conversion and product selectivity. The effect depended on both alkali type and loading. The catalyst with 0.8 wt% K gave the best result at 250 °C. It reached 14.7% CO₂ conversion, 78.3% methanol selectivity, and a methanol space–time yield of 468.5 g_MeOH kg_cat⁻¹ h⁻¹. CO selectivity decreased from 28.6% on the unpromoted catalyst to 15.9% after K addition. This result shows that K reduced the reverse water–gas shift reaction and directed more carbon toward methanol. The effect of alkali loading was not linear. Low loadings caused only small changes in surface properties, while loadings above 1.5 wt% lowered methanol production. The activity and basic-site results are shown in Fig. 1. Ali et al. (2026) also found that K improved CO₂ adsorption, Cu reduction, and methanol production over Cu/ZnO/Al₂O₃. Their results also showed that the preparation method changed the role of K. The present study confirms that alkali loading must be carefully controlled because excess promoter can reduce activity (Ali et al., 2026).

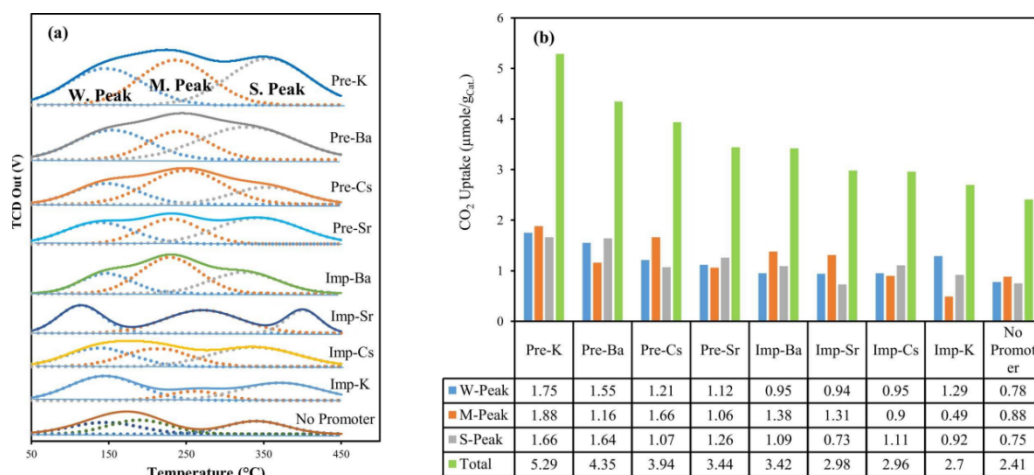


Fig. 1. Effect of alkali type and loading on CO₂ conversion, methanol selectivity, space–time yield, and surface basicity.

3.2 Balance between Basic Sites and Exposed Cu Sites

CO₂-TPD showed that K mainly increased the number of medium-strength basic sites. Their density rose from 186 $\mu\text{mol g}_{\text{cat}}^{-1}$ on Cu–ZrO_x to 312 $\mu\text{mol g}_{\text{cat}}^{-1}$ on the 0.8 wt% K catalyst. These sites adsorbed CO₂ strongly enough to form reactive surface species at the reaction temperature. However, they did not hold CO₂ as stable carbonate species. Higher K loadings increased the amount of strongly adsorbed CO₂, but methanol production decreased. H₂ chemisorption also showed fewer exposed Cu sites when the alkali loading exceeded 1.5 wt%. Thus, higher basicity alone did not improve activity. The catalyst required enough basic sites for CO₂ adsorption and enough open Cu sites for H₂ splitting. Cs caused stronger surface coverage because of its larger ionic size, while Na caused a smaller change in basic-site strength. K gave the best balance between these effects. Liang et al. (2026) also found that the effect of alkali promotion depended on local promoter–interface contact rather than only on changes in metal charge.

3.3 Surface Formate and Adsorbed CO Species

In situ DRIFTS showed stronger bands at 1582 and 1365 cm^{-1} after moderate K addition. These bands were assigned to surface formate species. Their higher intensity shows that K increased the amount of CO₂-derived intermediates near Cu–ZrO_x boundary sites. At the same time, the band from linearly adsorbed CO on Cu became weaker. This change agrees with the lower CO selectivity measured during reaction. The 0.8 wt% K catalyst therefore promoted formate formation and reduced CO build-up. At higher K loadings, the formate bands remained strong, but methanol production decreased. This result suggests that part of the formate became less reactive because hydrogen supply from Cu was limited (Liang et al., 2026; Turgut & Dincer, 2026). The DRIFTS spectra and kinetic results are shown in Fig. 2. Turgut et al. (2026) identified fast and slow formate species on Cu/ZrO₂. The fast species reacted about 65 times faster than the slow species. Their study shows that a strong formate band does not always indicate a high methanol rate. The position of formate and the supply of active hydrogen are also important.

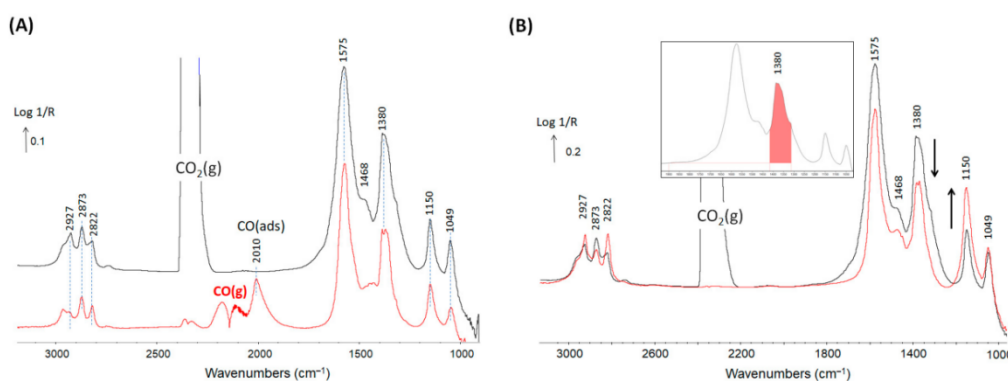


Fig. 2. In situ DRIFTS spectra and kinetic behavior of unpromoted and K-promoted Cu–ZrO_x catalysts.

3.4 Kinetic Role of the Acid–Base Balance

The apparent activation energy for methanol formation decreased from 72.8 to 57.6 kJ mol^{−1} after adding 0.8 wt% K. This decrease shows that moderate K loading made the hydrogenation of CO₂-derived intermediates easier. The CO₂ reaction order was 0.38, which suggests that CO₂ coverage was already high on the promoted surface. In contrast, the H₂ reaction order was 0.94. Methanol formation therefore remained strongly dependent on hydrogen supply. These results explain the loss of activity at high alkali loading. Excess alkali increased CO₂ adsorption but covered Cu sites needed for H₂ splitting. The best catalyst did not have the highest total basicity. It had enough medium-strength basic sites and enough exposed Cu sites. This result shows that alkali promoters do more than increase CO₂ uptake (Bao & Wang, 2026). They change the balance between CO₂ adsorption and H₂ activation. The catalyst should therefore be designed to balance these two functions rather than maximize only one of them.

4. Conclusion

Alkali addition changed the surface acid–base balance and product selectivity of Cu–ZrO_x catalysts during CO₂ hydrogenation. The catalyst with 0.8 wt% K gave the best result at 250 °C. It reached 14.7% CO₂ conversion, 78.3% methanol selectivity, and a methanol space–time yield of 468.5 g_MeOH kg_cat^{−1} h^{−1}. K addition increased the number of medium-strength basic sites from 186 to 312 μmol g_cat^{−1}. It also reduced CO selectivity from 28.6% to 15.9%. In situ DRIFTS showed stronger formate bands and weaker bands from linearly adsorbed CO after K addition. The apparent activation energy for methanol formation decreased from 72.8 to 57.6 kJ mol^{−1}. These results show that moderate K loading improves CO₂ adsorption and formate hydrogenation while keeping enough Cu sites available for H₂ splitting. In contrast, alkali loadings above 1.5 wt% covered Cu sites and reduced methanol production. Methanol selectivity therefore depends on a suitable balance between medium-strength basic sites and exposed Cu sites. Total CO₂ uptake alone cannot explain catalyst performance. These findings may help guide the design of promoted Cu catalysts for methanol and other C₁ oxygenates. However, this study was limited to laboratory-scale tests, one Cu–ZrO_x composition, and a narrow pressure range. Further work should include longer stability tests, wider reaction conditions, and operando studies under practical conditions.

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