Research Article

The behaviors of ultra-low-gold-loaded catalysts (Au/CeO$_2$) for CO oxidation in the presence of water on the catalysts

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ABSTRACT

The catalytic behavior of ultra-low-gold-loaded Au/CeO$_2$ during CO oxidation was studied using HRTEM, TGA, *in-situ* FTIR, CO–TPD, O$_2$–TPD, and O$_2$–TPO. Herein, water, which facilitates CO oxidation, is present on the catalyst rather than obtained from the reactant gas. The experimental results show that the presence of water on the catalyst enhances the adsorption and activation of O$_2$ to produce O$_{act}$ on the catalyst surface, resulting in excellent catalytic activity. Different reaction pathways for CO oxidation over Au/CeO$_2$ may be present; however, the dominant pathway is influenced by the species on the catalyst surface.

1   Introduction

Au-based catalysts are commonly used in CO oxidation due to their superior activities [1–11], but the high price and low availability of Au limit their application. Previously, we reported that our ultra-low-gold-loaded catalysts are quite reactive, some of which could oxidize 70% CO at ambient temperature, even though the amount of Au loaded was only 0.06 wt.% [12].

The main reason can be attributed to the contribution of water. Herein, to facilitate CO oxidation, water is present on the catalyst rather than being supplied from the humid reactant gas. Many reports have focused on the catalytic role of water from the humid reactant gas [13–15], while few studies have mentioned the water contained in the catalyst. Haruta and Date reported that the amount of water absorbed on the catalyst influences the activity, rather than the water

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content in the gas phase [13]. Consequently, we investigated the cases in which the catalyst already possesses water, thereby omitting the necessity of water adsorption from the humid gas phase.

Although extensive studies have shown that the presence of water is crucial to obtain excellent catalytic activity for CO oxidation, the intrinsic role of water in this process remains unclear. Haruta et al. considered that water not only activates molecular O_2, but also benefits the decomposition of carbonate-like species via the transformation of stable to unstable species [16]. In contrast, Goodman et al. proposed that the promotional effect of water can only be rationalized by its effects on O_2 adsorption and activation, and the appearance of carbonate-like species inhibits CO oxidation [17]. From the active debate, the consensus of the adsorption and activation of O_2 by water was reached. Liu et al. provided DFT calculations showing that hydroxyl (–OH) groups play a key role in O_2 adsorption on $TiO_2(110)$ [18]. Bongiorno and Landman used the first-principles calculations to demonstrate that an adsorbed H_2O molecule serves as an "attractor" of O_2 to its vicinity [19]. Based on a DFT and kinetic isotope effects study, it was concluded that H_2O-mediated O_2 activation occurs via the formation of hydroperoxy (–OOH) intermediates, which readily react with CO and account for the remarkable reactivity [20, 21]. However, to date there is no direct experimental evidence to validate the persistent speculation, which was obtained theoretically [18–21] and by exclusive methodology [17]. How the water changes during the activation process, and how to directly prove the existence of the proposed active –OH or –OOH groups remain unknown. Furthermore, the greatest difference between the two opinions is in regards to the role of carbonate-like species resulting from the reaction between CO and –OH or –OOH groups. It is unknown whether the carbonate-like species contribute to or inhibit the activity. Moreover, it remains unknown whether the rate-determining step for CO oxidation is the appearance of carbonate species or the activation of O_2.

In-situ Fourier transform infrared (FTIR) spectroscopy is the most widely used technique for studying reaction pathways. In order to determine directly how water improves the catalytic activity, the reaction pathways for CO oxidation were monitored in the presence of water on the catalysts by *in-situ* FTIR. Water existing on the catalyst, rather than supplied from the reactant gas, plays an important role in detecting the delicate changes in the signals of –OH groups by *in-situ* FTIR. When water is supplied from the reactant gas, it is very difficult to investigate changes in the –OH region by *in-situ* FTIR because the environmental water content is much higher than that adsorbing on the catalyst, which conceals the delicate signal changes of the surface –OH groups. Our study of water possessed by the catalyst itself circumvents this problem. Furthermore, we used CO-temperature-programmed desorption (TPD), O_2–TPD, and O_2-temperature-programmed oxidation (TPO) to characterize the catalysts, investigate the role of carbonate species, and determine the correlation between water and O_2.

2 Experimental

2.1 Catalyst preparation

In this work, different CeO_2 support structures were prepared by direct thermal decomposition of $Ce(NO_3)_3 \cdot 6H_2O$ at 873 and 1,073 K under atmospheric conditions. Au (0.1 wt.%) was introduced to the mentioned CeO_2 supports by a deposition precipitation method. An appropriate quantity of CeO_2 support was suspended in de-ionized water to produce a suspension. The pH value of the suspension was raised to 9 by NaOH and then the base suspension was heated to 343 K. An aqueous solution of $HAuCl_4$ was then introduced and reacted for 60 min. The resulting suspension was cooled and filtered. The solid obtained was washed thoroughly and dried at 333 K for 16 h without further calcination to produce the catalyst. Such a low heat-treatment temperature allows residual water on/in the catalysts. Using different CeO_2 supports, different catalysts, Au/CeO_2-873 and Au/CeO_2-1073, was obtained.

For comparison, similar pretreatments were performed on the CeO_2-873 and CeO_2-1073 supports without the use of $HAuCl_4$. The supports were stirred in alkaline water (pH = 9) at 343 K for 60 min, dried at 333 K for 16 h with some water present on/in the support, and named h-CeO_2-873 and h-CeO_2-1073, respectively.

2.2　Measurement of catalytic activity

Activity measurements were performed in a quartz tubular fixed–bed reactor with 0.2 g of the catalyst per pass under atmospheric pressure, 298 K, and GHSV = 18,000 h^{-1}; the composition of the reactant gas was 1% CO, 1% O_2, and 98% N_2.

2.3　Catalyst characterization

The HRTEM images of the samples were obtained using a Phillips Analytical FEI Tecnai 30 electron microscope operating at 300 kV. The samples were ground to a fine powder and mixed with acetone to create a suspension. A drop of the suspension was placed on a lacey carbon nickel grid, and subsequently dried at room temperature. In order to examine the Au particle size, the same method was used to prepare the above two catalysts but the Au content was increased from 0.1 to 1 wt.%.

The water content of the studied catalysts was evaluated using an SDT-Q600 instrument. Samples of approximately 6.5 mg were used in the TGA analyses. The temperature was increased to 850 K at a heating rate of 10 K/min. Weight and temperature data were recorded using TGA software.

In-situ FTIR investigations were performed in a Nicolet Nexus. This setup allows measurement in a continuous flow of gas mixtures, equaling those used in the activity measurements (1% CO, 1% O_2, and 98% N_2), and at 298 K. The samples, which were in self-supported pellets without KBr, were added to the *in-situ* reaction cell units. The sample surfaces were cleaned by vacuum pumping and then exposed to the reactant gas. The FTIR data were reported as Kubelka-Munk units, and 400 scans (nominal resolution 8 cm^{-1}) were co-added for one spectrum. The background spectra were measured in the third minute after the reactant gas had flowed through the catalyst rather than in the vacuum system, therefore any peak or valley was related to the amount of corresponding species increasing or decreasing during the reaction period. If the surface species do not change, the FTIR spectra show a straight line.

CO–TPD and O_2–TPD: Temperature-programmed desorption of CO and O_2 experiments were performed in a quartz microreactor connected to a mass spectro-meter (MS, Hiden QIC-20). The fresh catalyst was first pretreated under CO or O_2 at room temperature for 1 h (30 mL/min), and purged with Ar for 1 h. The temperature was then ramped to 1,073 K linearly (10 K/min) in a carrier Ar gas introduced at a rate of 10 mL/min.

O_2–TPO: Temperature-programmed oxidation of O_2 experiments was performed in a quartz microreactor connected to an MS (Hiden QIC-20). After reacting 1 h, the catalyst was treated under O_2, and the temperature was ramped from room temperature to 1,073 K linearly (10 K/min) in a carrier Ar gas introduced at a rate of 10 mL/min.

3　Results and discussion

3.1　Physicochemical properties of ultra-low-gold-loaded catalysts

We have previously reported that the introduced Au (0.1 wt.%) remained at 0.06 wt.% on the surface or the subsurface layers of Au/CeO$_2$-873 and Au/CeO$_2$-1073; the Au particle size and specific surface area were 4.8 nm and 66 m^2/g, respectively, for Au/CeO$_2$-873, and 5.1 nm and 6 m^2/g, respectively, for Au/CeO$_2$-1073 [12]. With the increase in support calcination temperature, the respective Au particle sizes remain similar to the previously reported values; however, the specific surface areas drop significantly (Fig. 1). Since the catalysts were prepared by depositing Au on a preformed ceria support and dried at 333 K without further heat-treatment, the effect of particle size on the catalytic activity is negligible.
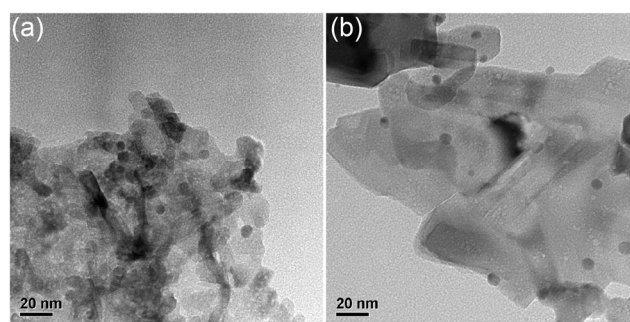

Figure 1　High-resolution transmission electron microscopic images of the catalysts with 1 wt.% Au content: (a) Au/CeO$_2$-873 and (b) Au/CeO$_2$-1073.

The water content of the studied catalysts was evaluated using TGA. The results show that after drying at 333 K, Au/CeO$_2$-873 and Au/CeO$_2$-1073 contain 2.39 and 0.53 wt.% water, respectively (Fig. 2). The relatively higher water content of Au/CeO$_2$-873 can be attributed to the higher specific surface area.

3.2 Reaction pathway of ultra-low-gold-loaded catalyst, Au/CeO$_2$-873

Herein, the special reaction pathways of the ultra-low-gold-loaded catalysts for CO oxidation with water on the catalysts were monitored by *in-situ* FTIR. In the carbonyl (OCO–) region, 1,588 cm^{-1} is assigned to
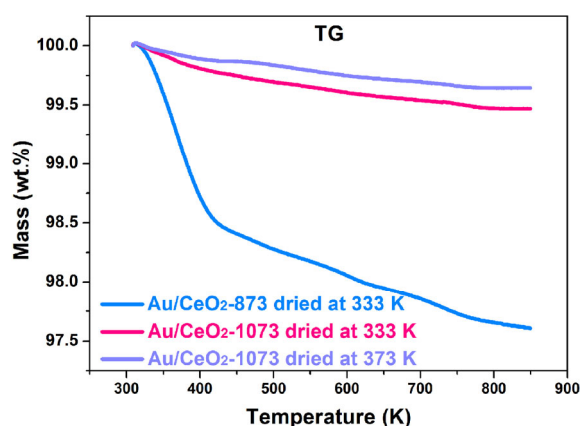
Figure 2 TGA tests for Au/CeO$_2$-873 and Au/CeO$_2$-1073 dried at 333 K, and Au/CeO$_2$-1073 dried at 373 K.

the bidentate formate, and 1,369 and 1,292 cm^{-1} are related to the carbonate-like species in the water-gas shift (WGS) reaction [22]. For the pure h-CeO$_2$-873 support, peaks are observed at 1,588, 1,369, and 1,292 cm^{-1} and remain constant (Fig. 3(b)), indicating that CO adsorbs on the hydroxylated support surface, forming formate and carbonate-like species even without Au. In contrast, for the Au/CeO$_2$-873 catalyst, the intensities of the 1,588, 1,369, and 1,292 cm^{-1} peaks increase rapidly with time during the first 35 min of the reaction, but level off thereafter (Fig. 4(b)). Such formation rates are identical to the CO conversion rate during the activity test (Fig. 4(a)), inferring that the peaks represent reaction intermediates during the CO oxidation. If these formate and carbonate-like species were formed by re-adsorption of the reaction product, CO$_2$, on the surface [23], the corresponding peaks would not be detected on the pure h-CeO$_2$-873 support, which shows no CO oxidation activity at 298 K (Fig. 3(a)).

The adsorption behavior of CO on the h-CeO$_2$-873 support and Au/CeO$_2$-873 catalyst was further investigated by CO–TPD (Fig. 5). The main signal is CO$_2$ rather than CO, suggesting CO can be oxidized to CO$_2$ during the desorption process. The results show that h-CeO$_2$-873 has the ability to absorb CO, but the adsorption capacity is much lower than that of
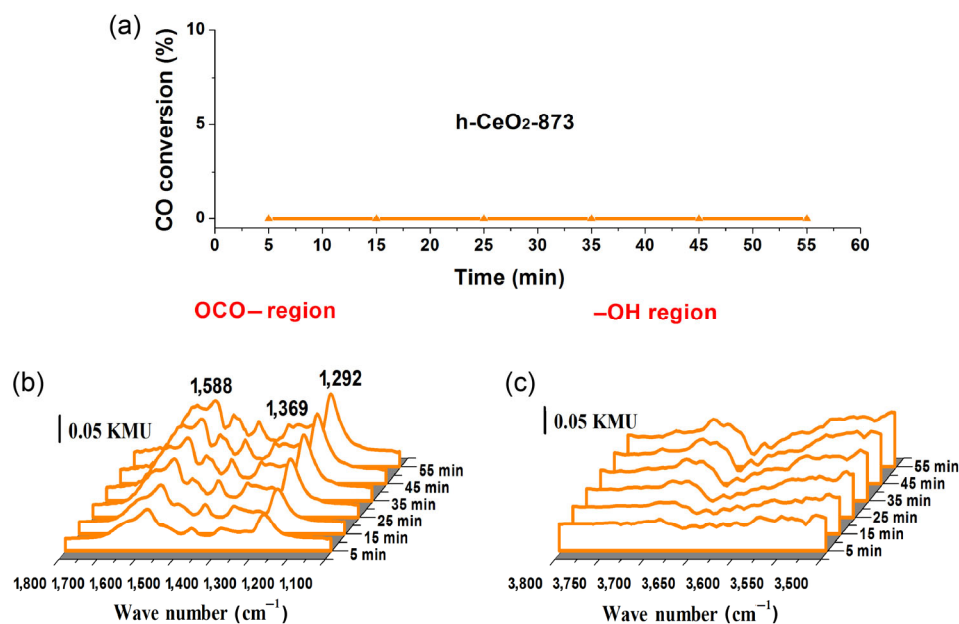
Figure 3 Activity (a) and series of *in-situ* FTIR spectra (b) and (c) obtained during the CO oxidation at 298 K over 55 min on h-CeO$_2$-873.
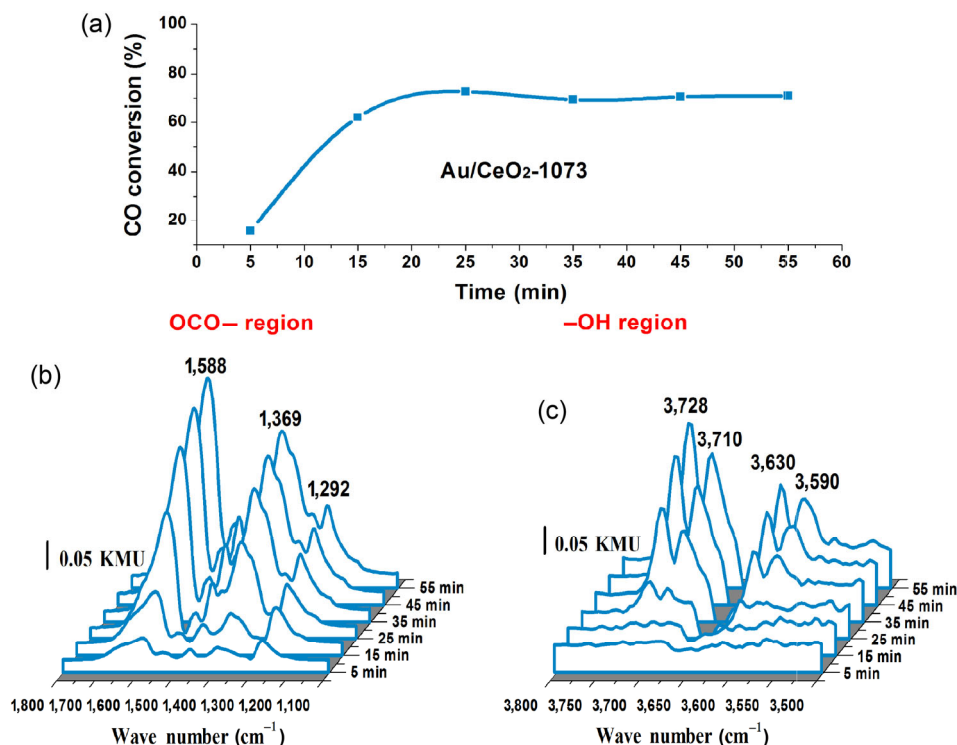
Figure 4 Activity (a) and series of *in-situ* FTIR spectra (b) and (c) obtained during the CO oxidation at 298 K over 55 min on Au/CeO$_2$-873.
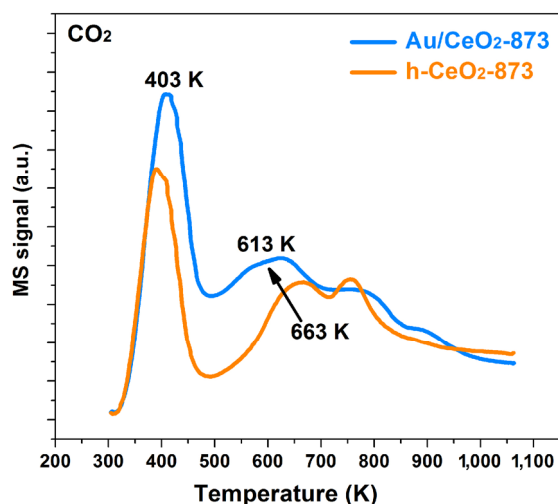

Figure 5 Mass spectra of CO$_2$ during CO–TPD on Au/CeO$_2$-873 and h-CeO$_2$-873.

Au/CeO$_2$-873. In addition, since Au weakens the Ce-O bond to increase the lattice oxygen mobility [24], the CO$_2$ desorption peak at 663 K on h-CeO$_2$-873 migrates to 613 K on Au/CeO$_2$-873. Moreover, although the hydroxylated support, h-CeO$_2$-873, adsorbs CO to form formate and carbonate-like species as Au/CeO$_2$-873 does, it shows no CO oxidation activity at 298 K.

Therefore, we speculate that the excellent catalytic activity of Au/CeO$_2$-873 is governed by key factors other than the formate and carbonate-like species.

In the –OH region, the Au/CeO$_2$-873 peaks at 3,590, 3,630, 3,710, and 3,728 cm^{-1} (Fig. 4(c)), representing active –OH groups [22, 25], have similar appearance rates as formate and carbonate-like species, but few changes are observed for h-CeO$_2$-873 in the –OH region (Fig. 3(c)). Meanwhile, the water-bending mode at 3,650 cm^{-1} decreases and forms a valley for Au/CeO$_2$-873. Comparison of the FTIR and CO–TPD results of h-CeO$_2$-873 and Au/CeO$_2$-873 shows that a small amount of Au loaded on the surface not only enhances the adsorption of CO on the catalyst, but also activates H$_2$O to produce new –OH groups located at different position.

Although CO and H$_2$O are present simultaneously, the WGS reaction requires a significantly higher temperature to convert CO to CO$_2$, thereby excluding the possibility of the WGS reaction during CO oxidation in the presence of H$_2$O at room temperature. The only way to produce the active –OH group just left the reaction between H$_2$O and O$_2$. H$_2$O activates O$_2$ by

two methods. One was proposed by Haruta et al. [16]: $O_2 + H_2O \rightarrow 2{-}OH + O_{act}$. The other was reported by Ojeda et al. [20]: $O_2 + H_2O \rightarrow {-}OOH + {-}OH$. O_2 could be activated by H_2O to produce active $-OH$ groups, $-OOH$ groups, and O_{act} at the perimeter interfaces between Au and the support. More facile oxygen adsorption in the presence of H_2O was also corroborated by DFT calculations [18]. O_{act} could directly react with the Au bonded CO (Au–CO) to produce CO_2, while the active $-OH$ and $-OOH$ groups could react with Au–CO to form intermediates such as formate $(Au{-}COOH)_{interface}$ and carbonate-like $(Au{-}CO_3H)_{interface}$ species. These intermediates forming at the perimeter interfaces are easily converted into CO_2 by the attack of O_{act}. Boccuzzi et al. performed CO oxidation over Au/TiO_2 with $C^{16}O$ and $^{18}O_2$ in the presence of $H_2^{16}O$ and observed only the formation of $C^{16}O^{18}O$. This excluded the participation of oxygen from either the support or H_2O, but indicated that the promotional effect of H_2O may be associated with the dissociation of O_2 [26]. Although O_{act} was not detected in this work, our experimental results from the water side shed light on the relationship between water and O_2.

However, the formation of formate $((-COOH)_{support})$ and carbonate-like $((-CO_3H)_{support})$ species on the support, observed in the OCO- region of h-CeO_2-873, remain stable due to the lack of Au to produce O_{act}. In the WGS reaction, decomposition of the $(-COOH)_{support}$ and $(-CO_3H)_{support}$ species requires a much higher temperature, which is also due to the lack of an O_{act} source in the reactant gas. In addition, without the addition of O_2 in the CO–TPD experiment system, the CO_2 desorption peak at 403 K does not shift to room temperature, as shown in the activity test over Au/CeO_2-873.

Consequently, there are two locations where formate and carbonate-like species form on the Au/CeO_2-873 surface: (1) on the interfaces between the Au and support, and (2) solely on the support. The former catalysts could act as reaction intermediates to produce CO_2 by the attack of O_{act}. The latter would remain stable on the support and reduce the O_2 adsorption capacity of CeO_2, and finally inhibit the catalytic activity. In order to prove our argument, a comparative experiment was designed. CO–TPD and CO_2–TPD were used for the fresh Au/CeO_2-873, and O_2–TPO was

applied for Au/CeO_2-873 after reacting 1 h.

Figure 6 shows that CO_2 signals are detected in each of the three cases. The peak around 400 K is detected in all cases, but there is a small shoulder peak at 335 K and peaks at 527 and 605 K in the O_2–TPO spectrum, which are not detected in the CO_2–TPD and CO–TPD spectra. These three special CO_2 desorption peaks can be attributed to the decomposition of $-COOH$ and $-CO_3H$ species, which are produced by co-adsorption of the active $-OH$ and $-OOH$ groups, as well as the CO on the catalyst surface. In the cases of CO–TPD and CO_2–TPD without O_2 addition, these three CO_2 desorption peaks are not found because H_2O in the catalyst is unable to react with O_2 to produce active $-OH$ and $-OOH$ groups. However, the peak at 335 K represents the decomposition of intermediate $(Au{-}COOH)_{interface}$ and $(Au{-}CO_3H)_{interface}$ species by the attack of O_2, and the peaks at 527 and 605 K represent thermal decomposition of the $(-COOH)_{support}$ and $(-CO_3H)_{support}$ species at high temperature.

These comparative experiments demonstrate that during the reaction process, some formate and carbonate-like species can be produced on the catalyst surface because of co-adsorption of the active $-OH$ and $-OOH$ groups, as well as CO. Therefore, the formation rates of the species in the OCO– region remain synchronized with those in the $-OH$ region. Meanwhile, the excellent CO activity is determined by the promotion of O_2 activation by H_2O ($O_2 + H_2O \rightarrow 2{-}OH + O_{act}$ and $O_2 + H_2O \rightarrow {-}OOH + {-}OH$), since the formation rates of the species in the OCO– region
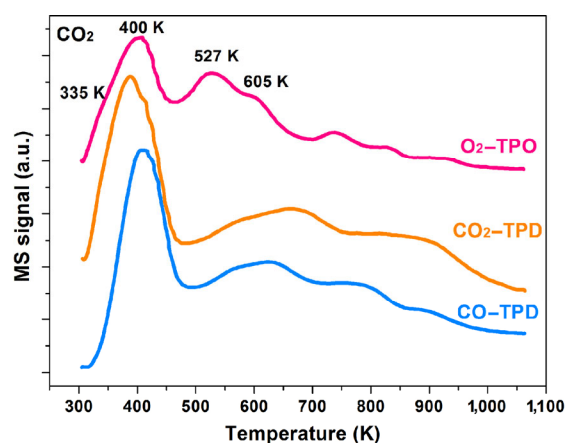

Figure 6 Mass spectra of CO_2 during CO–TPD and CO_2–TPD for fresh Au/CeO_2-873, and O_2–TPO for Au/CeO_2-873 after reacting 1 h.

and in the –OH region are also identical to the CO conversion rate during the activity test. However, only the (Au–COOH)$_{interface}$ and (Au–CO$_3$H)$_{interface}$ species forming on the interfaces are reaction intermediates, and the others would remain stable on the support, such as (–COOH)$_{support}$ and (–CO$_3$H)$_{support}$.

3.3 Reaction pathway of ultra-low-gold-loaded catalyst, Au/CeO$_2$-1073

Figures 7 and 8 show the *in-situ* FTIR results of h-CeO$_2$-1073 and Au/CeO$_2$-1073. No significant changes occur on h-CeO$_2$-1073 in the OCO– (Fig. 7(b)) and –OH (Fig. 7(c)) regions, and therefore show no CO oxidation (Fig. 7(a)). Figure 2 shows that Au/CeO$_2$-873 and Au/CeO$_2$-1073 dried at 333 K contain 2.39 and 0.53 wt.% water, respectively. It is then speculated that the water content in h-CeO$_2$-1073 is much lower than h-CeO$_2$-873, and therefore the FTIR intensities of the (–COOH)$_{support}$ and (–CO$_3$H)$_{support}$ species forming on the h-CeO$_2$-1073 support are weaker than those of h-CeO$_2$-873 are. Meanwhile, without the addition of Au in h-CeO$_2$-1073, H$_2$O and O$_2$ lack the interface to produce new –OH groups and O$_{act}$.

Interestingly, no obvious peaks are detected for Au/CeO$_2$-1073 in the OCO– region (Fig. 8(b)), while the peak intensities in the –OH region slightly increase and remain stable after 15 min (Fig. 8(c)). This suggests that the catalyst experiences a different reaction

pathway, in which formate or carbonate-like species forming on the interface are unnecessary and Au-CO directly reacts with O$_{act}$ to produce CO$_2$. Based on the XPS results [12], only Au^0 is detected on Au/CeO$_2$-1073, but 16% Au$^{\delta+}$ is found on Au/CeO$_2$-873. An inference can be drawn that Au$^{\delta+}$ is the requisite species to form the formate and carbonate-like species, which is consistent with the WGS reaction mechanism. Regardless whether the Au^0 species act as spectators or contribute to the WGS activity, Au$^{\delta+}$ species have been accepted as active species to form reaction intermediates [22, 27].

We previously reported that Au/CeO$_2$-1073 shows poor oxidation of CO after drying at 373 K (CO conversion decreases from 35% to 10%) [12]. The TGA results show that the water content decreases from 0.53 to 0.35 wt.% (Fig. 2). Lack of the water-derived species makes it difficult to exhibit the promotional effects on molecular oxygen adsorption and activation. Au/CeO$_2$-873 is more active than Au/CeO$_2$-1073, however based on the XPS results, it can be inferred that a large amount of Au$^{\delta+}$–OH remains on the Au/CeO$_2$-873 surface, and drying the catalysts at 373 K results in thermal decomposition of Au$^{\delta+}$–OH species or recombination of –OH groups such that Au$^{\delta+}$ species transform to Au^0. Thus, the changes in activity could be attributed to the effect of water or the Au^0/Au$^{\delta+}$ ratio. In contrast, Au^0 is the main Au
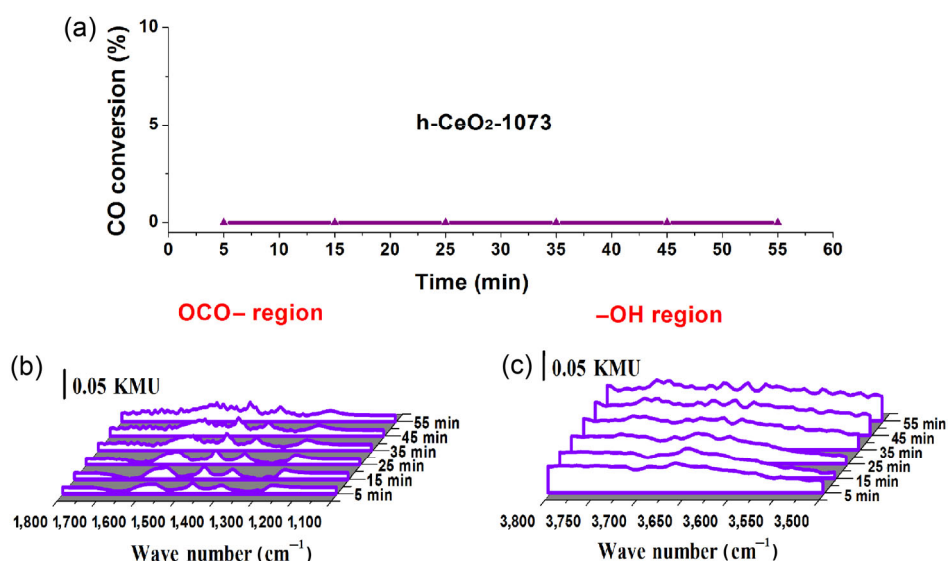

Figure 7 Activity (a) and series of *in-situ* FTIR spectra (b) and (c) obtained during the CO oxidation at 298 K over 55 min on h-CeO$_2$-1073.
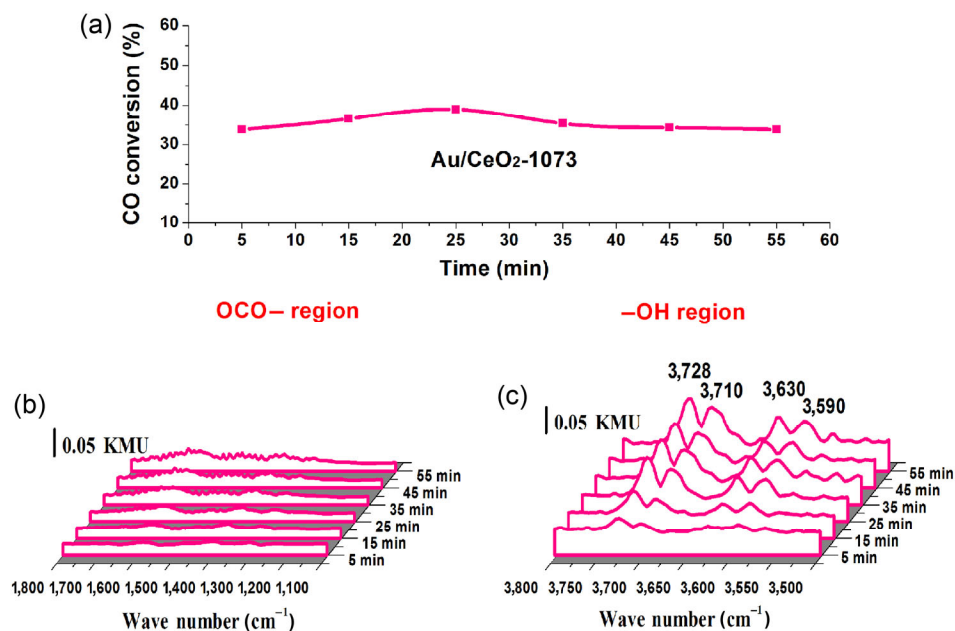
Figure 8 Activity (a) and series of *in-situ* FTIR spectra (b) and (c) obtained during the CO oxidation at 298 K over 55 min on Au/CeO$_2$-1073.

species on the surface of Au/CeO$_2$-1073, and sintering of Au particles does not occur at such low temperatures. Therefore, the change in activity can be chiefly attributed to the amount of water absorbed on the surface [12]. In order to understand the specific effect of O$_2$ and H$_2$O on CO conversion, O$_2$–TPD experiments were performed over Au/CeO$_2$-1073 dried at 333 K and 373 K.

The mass spectra of O$_2$ and H$_2$O in the O$_2$–TPD process are illustrated in Fig. 9. When the drying temperature is increased from 333 to 373 K, the amount of H$_2$O on/in the catalysts decreases significantly. In particular, the H$_2$O peak at 673 K nearly disappears in the case of Au/CeO$_2$-1073 dried at 373 K, which represents the chemisorbed water or the recombination of –OH groups. During the O$_2$ adsorption process, the following reactions occur: O$_2$ + H$_2$O → 2–OH + O$_{act}$ and O$_2$ + H$_2$O → –OOH + –OH. O$_{act}$ could be stored by CeO$_2$ and then desorbed as O$_2$ when the temperature increases. With the decrease of H$_2$O content, the amount of adsorbed O$_2$ is also reduced. In addition, when the catalyst is dried at 333 K, most of the O$_2$ tends to desorb at lower temperatures, due to the adsorption of O$_2$ at the metal support interfacial sites [28]. In contrast, most of the O$_2$ desorbs at higher temperatures when the catalyst is dried at 373 K,
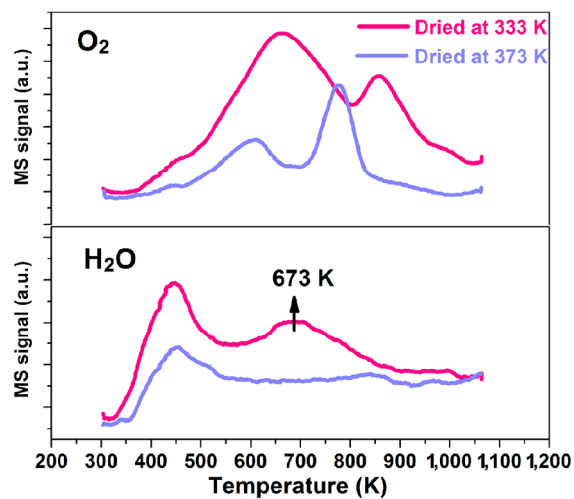

Figure 9 Mass spectra of O$_2$ and H$_2$O during O$_2$–TPD on the catalyst Au/CeO$_2$-1073 dried at 333 K and 373 K.

which is due to desorption of the chemisorbed O$_2$ molecules in the catalyst pores [26]. These results further demonstrate the promotional effect of water on the adsorption and activation of O$_2$.

3.4 Effect of O$_{act}$, H$_2$O, and –OH groups on the catalyst activity

Most of the previously reported catalysts applied in low temperature CO oxidation had higher Au loadings (>1 wt.%) than those employed in the current study.

However, the reaction activity in this study was found to improve when the catalyst possesses water on its surface, even though the Au content is less than 0.1 wt.%. These findings lead to the conclusion that O_{act} greatly contributes to the activity, and the interfaces between Au and the support supply a platform to produce O_{act}. The addition of H_2O accelerates the adsorption and activation of O_2, and –OH groups are the byproducts of the process. However, –OH groups can react with Au–CO to form intermediates, such as $(Au–COOH)_{interface}$ and $(Au–CO_3H)_{interface}$ species, which remain stable, rather than decompose to CO_2, without the attack of O_{act}. These studies suggest the participation of –OH groups in CO oxidation, but O_{act} is the most important active species. Saavedra et al. evaluated the reaction kinetics and found that weakly adsorbed water increased the effective number of active sites rather than changing their inherent reactivity [21]. These studies show us that the CO_2 product may be obtained by two reaction pathways, but the more effective pathway of the two remains unclear. Since the surface areas, water amounts, and $Au^0/Au^{\delta+}$ ratios between Au/CeO_2-873K and Au/CeO_2-1073K are very different, their activities are difficult to compare. Therefore, it is difficult to analyze whether O_{act} attacks the formate and carbonate-like species, or directly reacts with Au–CO to produce CO_2. In addition, a suitable amount of water on the surface is crucial to obtain excellent activity. Too much water could cover the active sites and lead to the accumulation of stable carbonate-like species on the support, which all negatively affect the activity.

4   Conclusions

In summary, the *in-situ* FTIR combined with HRTEM, TGA, CO–TPD, O_2–TPO, and O_2–TPD experiments presented herein, provide a more direct approach to understanding the catalytic performance of ultra-low-gold-loaded catalysts possessing water for CO oxidation at ambient temperature. To the best of our knowledge, this is the first demonstration of the delicate signal changes of –OH groups on the catalyst surface using *in-situ* FTIR, which supplies experimental evidence for the changes in water during the reaction process. The superior catalytic activity can be rationally

explained because the appropriate water content in the catalysts themselves promotes O_2 adsorption and activation to produce O_{act} species. The CO_2 product may be obtained by two reaction pathways: (1) the decomposition of reaction intermediates on the perimeter interface by the attack of O_{act}, such as $(Au–COOH)_{interface}$ and $(Au–CO_3H)_{interface}$ species, and (2) the direct reaction between Au–CO and O_{act}. $Au^{\delta+}$ species are requisite to form the formate and carbonate-like species on the interface, therefore the contribution of each is dependent on the catalyst surface composition.

Au/oxide catalysts have attracted much attention in PEM fuel cells due to their excellent catalytic activities for the selective oxidation of CO. It is curious what will happen on the surfaces of catalysts that possess water in the presence of H_2. In the future, research into the behavior of Au/oxide catalysts with water for selective oxidation of CO will be conducted.

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