

Catalytically Active Gold: From Nanoparticles to Ultrathin Films

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ABSTRACT

Ordered gold (Au) mono- and bilayer structures have been synthesized on a highly reduced titania surface. The Au bilayer exhibits a significantly higher catalytic activity for carbon monoxide oxidation than does the Au monolayer structure. This is the first report of Au completely wetting an oxide surface and demonstrates that ultrathin Au films on an oxide surface have exceptionally high catalytic activity, comparable to the activity observed for Au nanoparticles. This discovery is a key to understanding the nature of the active site of supported Au catalysts.

1. Introduction

Since the discovery that nanosized gold particles, highly dispersed on metal oxide supports, are active catalysts for a variety of reactions,¹ numerous studies have addressed the structure and mechanisms associated with this activity.^{2–23} The size of the Au nanoparticles and the support properties have been shown to be critical to their unique catalytic activity.^{1–3,9,10,13,14,20} The active sites have been proposed to be at the interface between the Au nanoparticles and the oxide support. However, the size distribution and shapes of these nanoparticles on an oxide surface vary widely, and the structures, particularly at the metal–oxide interface, are generally not well-defined. Moreover, Au nanoparticles typically sinter rapidly under realistic catalytic conditions. Because of these complexities, the active site and structure of supported Au catalysts remain unclear. The recent synthesis of highly ordered Au mono- and bilayer structures supported on a highly reduced titania surface and the exceptionally high catalytic activity for CO oxidation observed for the bilayer structure^{9,10} are important milestones in defining the nature of the active site for supported Au catalysts. These ordered Au films are stable in ultrahigh vacuum (UHV) up to 900 K, much higher than 700–800 K where supported Au nanoparticles rapidly sinter. These studies illustrate the

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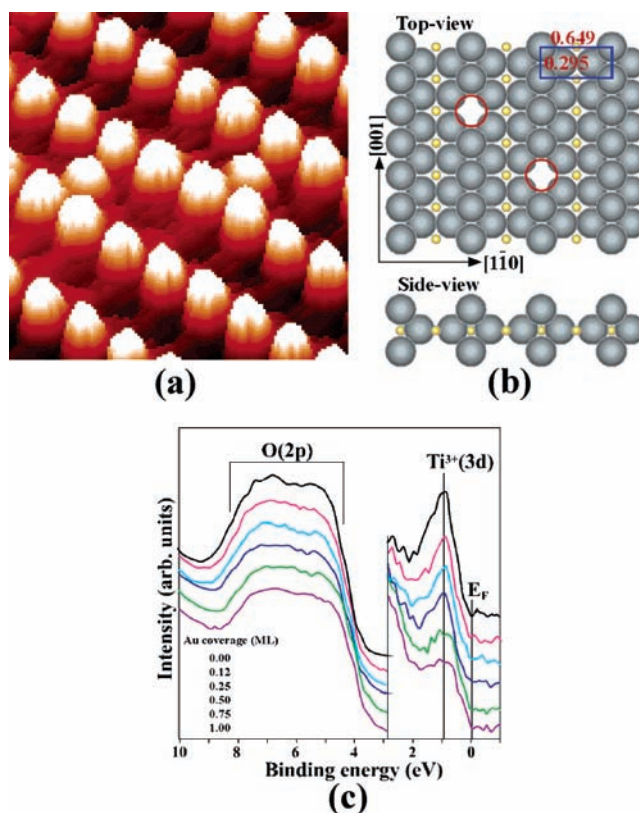


FIGURE 1. (a) A high-resolution STM image of $\text{TiO}_2(110)$, (b) a schematic structural model of $\text{TiO}_2(110)$ with empty circles indicating the surface oxygen vacancies, and (c) UPS spectra for a reduced $\text{TiO}_2(110)$ surface followed by deposition of various amounts of Au at room temperature.³⁴

importance of defects in the support structure for stabilizing Au nanoparticles and in the design of functional oxide supports for Au and other noble metal catalysts.

2. Surface Defects and Sinter-Resistant Supports

Defects on oxide surfaces are known to play a key role in the nucleation and growth of metal nanoparticles, as well as in defining their electronic properties. Therefore considerable work has focused on the characterization of surface defects and their interaction with metal atoms and particles, an especially useful atomic-level technique being scanning tunneling microscopy (STM). Figure 1a shows a high-resolution STM image of a single crystal rutile surface of titania, specifically, the $\text{TiO}_2(110)$ surface. The bright spots along the rows correspond to the surface five-coordinate Ti atom sites, coordinately unsaturated Ti cations, as shown in the schematic of Figure 1b. The additional bright spots between the ordered rows are surface oxygen vacancies, the so-called defects, as indicated by the red circles in Figure 1b. Defects of this kind can be created by sputtering with Ar^+ or annealing in UHV.²⁴ Such defects have been found to markedly affect

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the adsorption energy, particle shape, and the electronic structure of deposited Au nanoparticles and to influence their unique catalytic properties.^{2,9,14,17,19,25–32} Theoretical calculations have demonstrated that Au particles bind more strongly to a defect-rich surface compared with a defect-deficient surface and that significant charge transfer occurs from the titania support to the Au particles.^{2,9,30,31} High-resolution STM combined with density functional theoretical (DFT) calculations³¹ has confirmed that bridging oxygen vacancies are the active nucleation sites for Au particles on titania and that each vacancy site can bind approximately three Au atoms on average. The adsorption energy of a single Au atom on an oxygen vacancy site is more stable by 0.45 eV compared with the stoichiometric surface.³¹ Low-energy ion scattering (LEIS) has been used to examine the growth of Au on TiO₂(110).^{27,28} Two-dimensional (2-D) Au islands are initially formed up to a critical coverage that depends on the defect density of the titania surface, then three-dimension (3-D) particles start to form. The critical Au coverage at which transformation of Au particles from 2-D to 3-D occurs has been shown to be markedly dependent on the defect density, that is, the maximum coverage of 2-D domains correlates well with the surface defect density.^{27,28,33,34}

In recent work from our laboratory,³⁴ the surface oxygen vacancies on a highly reduced titania surface have been titrated by deposition of Au followed by ultraviolet photoemission spectroscopy (UPS). Emission from a Ti³⁺ electronic level at a binding energy of 0.9 eV is evident in the UPS data of Figure 1c. Note that on an oxygen vacancy site, two neighboring Ti atoms are reduced from Ti⁴⁺ to Ti³⁺. These Ti³⁺ surface defects can be completely reoxidized by exposure to oxygen.³⁵ Following Au deposition onto the reduced titania surface, a decrease in the intensity of the Ti³⁺ state is apparent, showing that Au initially nucleates at the defect sites. This suggests that Au atoms bond at oxygen vacancy sites, that is, bonding between Au and Ti³⁺. This observation is consistent with previous work showing that nanoparticles of Au on defect-rich titania are much more chemically active than on defect-deficient titania.^{17,19,28}

Figure 2a shows a STM image of 0.25 monolayers (one monolayer corresponds to one Au atom per surface Ti⁴⁺) of Au deposited on a TiO₂(110) single crystalline surface at 300 K followed by an anneal at 850 K for 2 min.² The atomically resolved TiO₂(110) surface consists of flat terraces with atom rows separated by ~0.65 nm. Au clusters with a relatively narrow size distribution and specific morphologies are imaged as bright protrusions. Schematics of the one-dimensional (1-D), 2-D, and 3-D Au structures with one, two, and three atomic layers in thickness are shown in Figure 2b–d.

Because of facile sintering as a deactivation mechanism of supported Au catalysts, considerable effort has focused on the design and synthesis of sinter-resistant oxide supports. A recent example is a Ti-doped SiO₂ film prepared on a Mo single-crystal surface.^{36,37} First, a well-ordered monolayer SiO₂ film with a well-defined $c(2 \times 2)$ low-energy electron diffraction (LEED) pattern was pre-

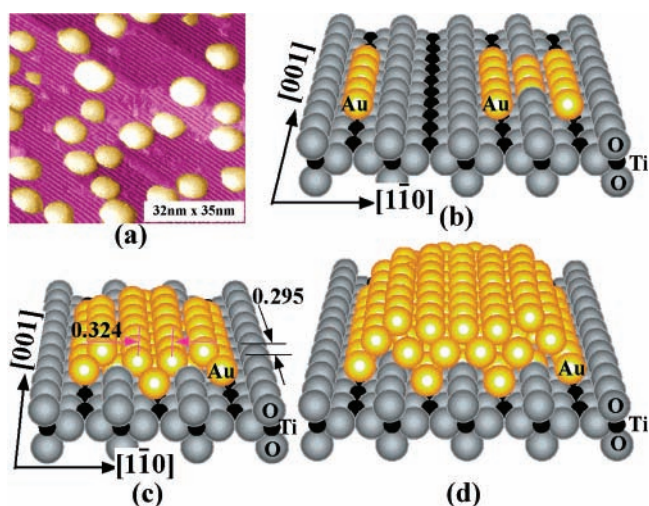


FIGURE 2. (a) A STM image of Au/TiO₂(110)-(1 × 1) with a Au coverage of 0.25 ML² and (b–d) schematic structural models for 1D, 2D, and 3D structures with two-atomic- and three-atomic-layers thick Au particles on the TiO₂(110). Adapted from ref 2 with permission from *Science* (<http://www.aaas.org>). Copyright 1998 American Association for the Advancement of Sciences.

pared on a single-crystal Mo surface. Ti was then deposited on the SiO₂ film at room temperature followed by oxidation at ~850 K and an anneal at ~1050 K. An 8% Ti doped surface is very flat and essentially free of 3-D Ti or TiO_x clusters, with isolated bright spots at the step edges and on the terraces as shown in Figure 3a. Ti was found to incorporate into the surface forming Ti–O–Si linkages as evidenced by high-resolution electron energy loss spectroscopy (HREELS)³⁶ and STM.³⁷ The average number density of isolated Ti atoms on the SiO₂ terrace from the STM images is estimated to be approximately $3.0 \times 10^{13}/\text{cm}^2$. With an increase in the Ti coverage to 17%, the surface remains flat with the formation of reduced, that is, TiO_x, 3-D islands on the SiO₂ terraces (Figure 3b). Au was found to nucleate primarily at the Ti defects when deposited on the 8% Ti-doped SiO₂ surface (Figure 3a). In contrast, Au primarily decorates the extremities of the TiO_x islands when deposited on the 17% Ti-doped SiO₂ surface (Figure 3b). Thermal sintering of Au particles on either of the Ti-doped surfaces was significantly inhibited compared with the corresponding sintering characteristics of Au on SiO₂.³¹ Adhesion between the Au particles and the support is clearly governed by the density of defects at the interface between the particle and the support. Indeed recent experiments and theoretical calculations show that Au on titania actually stabilizes the presence of oxygen vacancies at the particle–support interface.^{17,31,38}

Recently a highly ordered, reduced titania surface has been prepared on a Mo(112) substrate.^{9,36,39,40} The atomic resolved STM image and proposed structure for this reduced titania surface, designated as (8×2) -TiO_x, are shown in Figure 4a. In this model, seven Ti atoms decorate every eight Mo atoms along the Mo(112) trough, binding to the surface via Ti–O–Mo bonds and to each other via Ti–O–Ti linkages.^{9,40} On the rutile TiO₂(110) surface (see Figure 1b), the two Ti atoms nearest to an oxygen vacancy are reduced to Ti³⁺, whereas for the (8×2) -TiO_x surface,

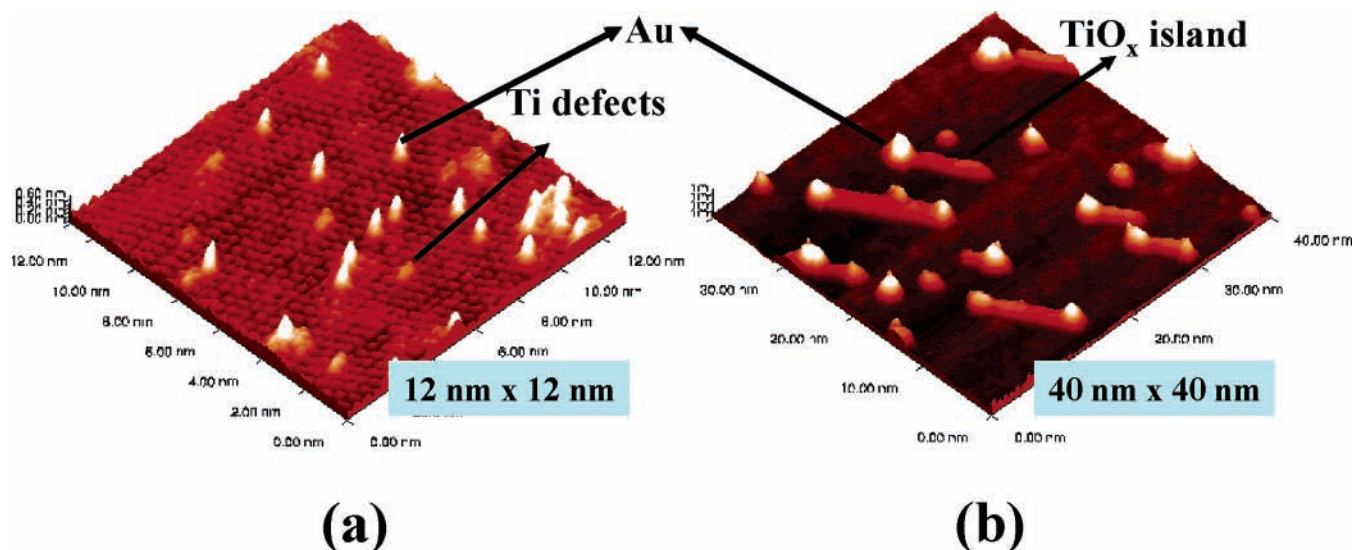


FIGURE 3. 3D STM images of (a) Au(0.04 ML)/TiO_x(8%)–SiO₂ and (b) Au(0.08 ML)/TiO_x(17%)–SiO₂ showing that both Ti defects and TiO_x islands play a role as nucleation sites for Au nanoclusters. Reproduced with permission from ref 37. Copyright 2004 American Chemical Society.

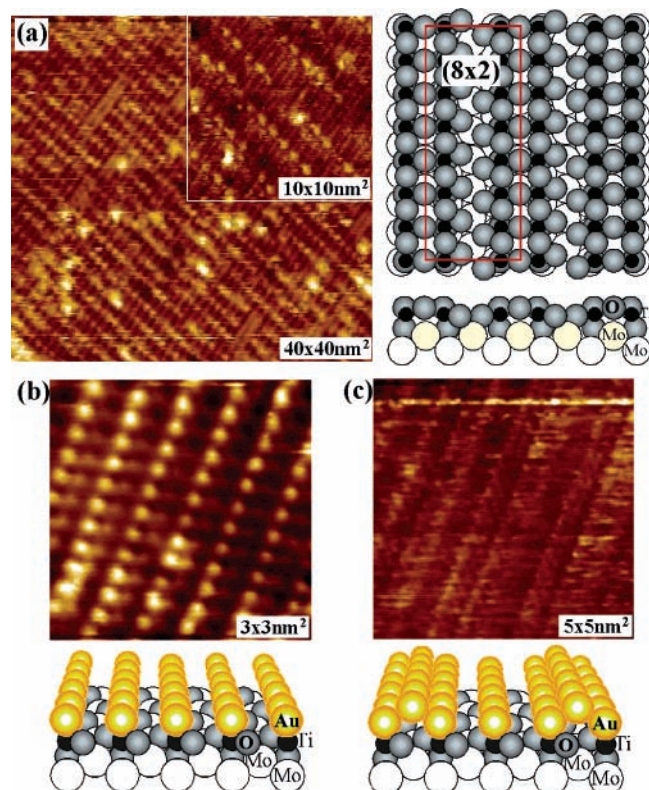


FIGURE 4. Structural model and atomic resolved STM image of (a) Mo(112)–(8 × 2)–TiO_x, (b) Mo(112)–(1 × 1)–(Au,TiO_x) and (c) Mo(112)–(1 × 3)–(Au, TiO_x). Reprinted with permission from *Science* (<http://www.aaas.org>), ref 9. Copyright 2004 American Association for the Advancement of Science.

there is a full monolayer of reduced Ti³⁺ sites.^{9,40} Accordingly strong binding between deposited Au and the TiO_x surface is anticipated. Indeed, upon deposition of Au onto this (8 × 2)–TiO_x surface followed by an anneal at 900 K, well-ordered Au monolayer and bilayer structures form with Au completely wetting the surface.⁹ The two ordered structures, designated as (1 × 1)–Au–TiO_x and (1 × 3)–

Au–TiO_x, respectively, are shown schematically in Figure 4b,c together with atomically resolved STM images.⁴¹ Temperature-programmed desorption (TPD) indicates that the Au–TiO_x interaction is much stronger compared with the Au–Au interaction.⁴¹

3. Active Au Catalysts: From Nanoparticles to Ordered Thin Films

The unique activities of highly dispersed nanosized Au particles on oxide surfaces^{1–14,42} are found to strongly correlate with the Au particle size; for example, the highest turnover frequency (TOF, reaction rate per surface Au site per second) occurs at a particle size of ~3 nm. A model catalytic system, Au/TiO₂(110), was used to investigate this unusual catalytic phenomenon under realistic reaction conditions.² Similar to results obtained for the corresponding high-surface-area supported Au/TiO₂ catalysts,¹ CO oxidation activities critically depend on the Au particle size, as shown in Figure 5a.² The maximum reaction rate, a turnover frequency of 2, was observed for a surface with Au particles of a mean particle size of ~3 nm and a particle thickness of two atomic layers as determined by STM.

The rates for catalytic CO oxidation over well-ordered Au mono- and bilayer structures of Figure 4b,c are shown in Figure 5b.⁹ At Au coverages less than 1 monolayer, where the Au particle morphologies correspond to 2-D domains, the rates are much less than the maximum. As the Au coverage is increased to greater than 1 monolayer, the rate increases sharply, then decreases markedly above ~1.5 monolayers of Au. The maximum reaction rate occurs at a Au coverage of ~1.3 monolayers, where the particle morphology corresponds to the Au bilayer structure. The rate, a TOF of 4, is higher than any previously reported rate for supported Au nanoparticles. These results show that extended ultrathin Au films on an oxide surface are as catalytically active as Au nanoparticles of

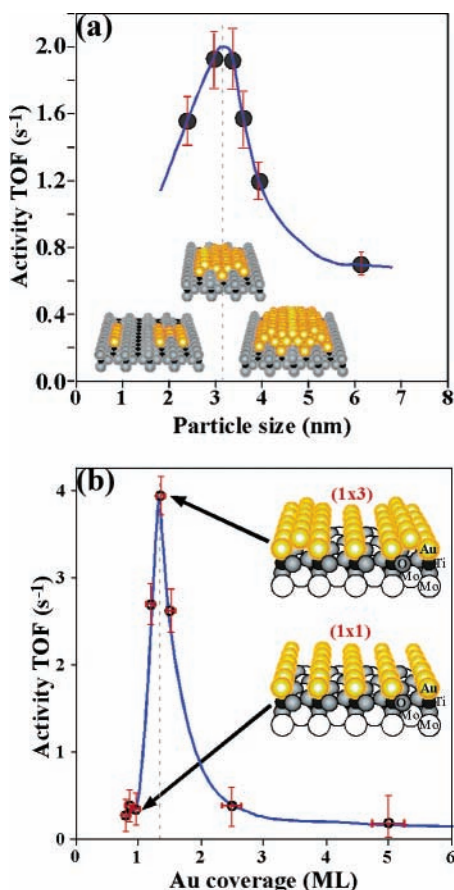


FIGURE 5. Catalytic activity for CO oxidation as a function of (a) particle size on the $\text{TiO}_2(110)$ at 353 K,² (b) Au coverage on the $\text{Mo}(112)-(8 \times 2)\text{-TiO}_x$ at room temperature.⁹ Reprinted with permission from *Science* (<http://www.aaas.org>), refs 2 and 9. Copyright 1998 and 2004 American Association for the Advancement of Science.

optimum diameter and that particle morphology is the key metric for activity, not simply particle diameter.

4. Active Site and Structure of Au Catalysts

Catalytically active Au has only been observed for Au particles less than 8 nm in diameter, and the observed activities are highly dependent on the support materials.^{1,43,44} Based on the above, the corner or edge sites at the perimeter/contact area of the interface between the Au particles and the support are purported to serve as a unique reaction site where the reactants are activated.^{1,44,45} However, the apparent lower catalytic rate measured for the monolayer compared with that for the bilayer (see Figure 5b),⁹ as well as that the catalytic rate decreases as the particle size decreases below 3 nm (with a thickness of two atomic layers) for supported Au nanoparticles (Figure 5a),² illustrates that synergism between the first and second layer is essential for the unique catalytic activity for supported Au nanoparticles. The rates for ordered bilayers, model nanoparticles with two atomic layers in thickness, and the very best high-surface-area supported catalysts are compared in Figure 6. The blue bars of the histogram are the computed rates based on total Au. The rates obtained for the ordered bilayers are approximately 1 order of magnitude higher than the rates

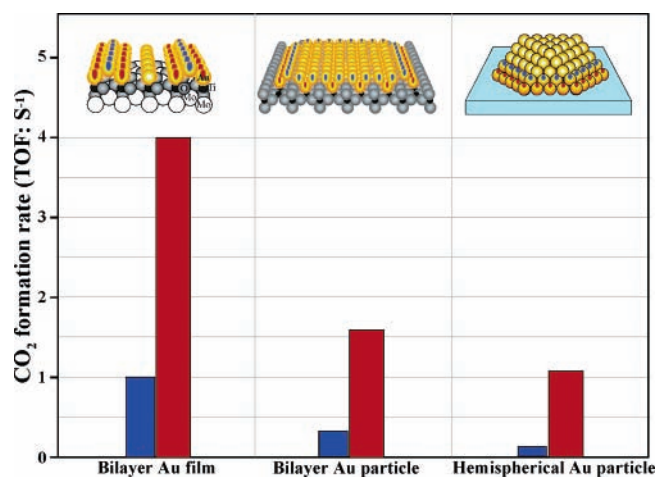


FIGURE 6. Comparison of catalytic activities for CO oxidation on the $\text{Mo}(112)-(1 \times 3)\text{-(Au,TiO}_x)$, $\text{Au/TiO}_2(110)$, and Au supported on high-surface-area TiO_2 with a mean particle size of ~ 3 nm. The inserts show structural models using red and blue marks to indicate the active sites.

for the high-surface-area supported catalysts. Assuming that a combination of the first and second layer Au atoms is the active site (see the inserts of Figure 6), the rates, computed on a per active site basis from the corresponding particle structure, become comparable as shown by the red bars of the Figure 6 histogram. It is noteworthy that on a per Au atom basis, the rates for the supported particles are decidedly lower than those for the Au bilayer. This may arise due to (1) the fact that various sizes and shape of the particles coexist on the surface, (2) an electronic effect caused by particle contact area, particle shape, etc., or (3) a steric effect in that the reactants have multidirectional access to the bilayer structure but only unidirectional access to the Au nanoparticles.

Another relevant question is whether the support is involved directly in activating reactant molecules. It is generally agreed that the support plays an important role in stabilizing and defining the morphologies and electronic properties of Au nanoparticles.^{2,9,14,17,19,28,31} The perimeter/contact area of the interface between the Au particles and the support has been proposed to serve as a unique reaction site where reactants are activated.^{1,44,46} From theoretical calculations, the support has been shown to play an active role in the bonding and activation of adsorbates bound to Au.^{47–49} Molina and Hammer⁴⁷ have proposed the active site to be low-coordinated Au atoms in combination with surface cations interacting simultaneously with an adsorbate. In ordered Au monolayer and bilayer structures described above, the Ti^{4+} of the support titania is not accessible to the reactants, since each surface Ti site binds directly to a Au atom located at the topmost surface.⁹ The exceptionally high catalytic activities for CO oxidation observed on ordered bilayer Au thus strongly suggest a Au-only CO oxidation pathway. This reaction pathway is supported by recent DFT calculations that show the reaction sequence for CO oxidation for Au-only surface sites on a TiO_2 supported Au nanoparticle to have a similar activation energy (0.36–0.40 eV) as that involving support cations.⁵⁰ Moreover, molecularly chemi-

sorbed oxygen on Au/TiO₂ is found to be stable at the surface^{48,51} and to react directly with CO to form CO₂ without requiring dissociation of O₂.⁵²

5. Origins of Exceptionally High Catalytic Activities for Nanosized Au Catalysts

The unique catalytic properties of supported Au nanoparticles have motivated extensive experimental and theoretical studies with the aim of elucidating the origin of the special activity. Unfortunately the data in the literature and the discussion vary widely; therefore the nature of the active Au species or structure or site remains unclear. In general, the origins of the catalytic activity of Au have been proposed to originate from one or more of three contributions: (i) presence of low coordination Au sites; (ii) charge transfer between the support and Au; (iii) quantum size effects.

Low-Coordination Au Sites. The size requirement for active Au particles is typically less than 8 nm in diameter. Because the density of corner, edge, or surface Au atoms relative to the number of total Au atoms in a particle increases with decreasing particle size, coordinatively unsaturated Au atoms at the corner, at the edge, and at the particle surface have been proposed to constitute the active sites.^{19,30,34,45,50,53} Indeed, the binding of CO and O₂ are demonstratively higher at the corner or edge sites than on the terrace or on the smooth surface.^{19,30,45} Moreover, DFT calculations show that oxygen and carbon monoxide can only adsorb on gold atoms with a coordination number less than 8 at a certain condition.⁵³ This was confirmed by CO adsorption on Au/TiO₂, Au/ZrO₂, and Au/FeO using infrared spectroscopy.^{54,55} The CO oxidation involves adsorption of CO and O₂; the presence of low-coordinated Au atoms was therefore regarded to be a key factor for the catalytic activity of Au nanoparticles.¹⁹ However, a lower catalytic activity is found for monolayer Au (coordination number of 3–4) compared with bilayer Au (coordination number of ~6 (see Figure 5b)).⁹ Furthermore for supported Au nanoparticles, the catalytic rate decreases as the particle size decreases below 3 nm although the relative densities of the corner or edge sites increase continuously with decreasing particle size (Figure 5a).² Therefore low-coordinated corner or edge sites alone are not the single factor upon which catalytic activity is dependent.

Charge Transfer between the Support and Au. The interaction between Au and the support alters the electronic structure of Au nanoclusters and promotes their catalytic activities for low-temperature CO oxidation. In particular, defects on the oxide support are thought to play a key role in anchoring the Au particles and in transferring electronic charge to Au, with these two effects in combination contributing to the special catalytic activity.^{2,6,9,17,19,27–34,56} The electronic state of Au nanoparticles can be probed using CO adsorption in combination with infrared spectroscopy. It has been shown that the ν_{CO} mode shifts to lower frequency on electron-rich Au clusters and to higher frequency on electron-deficient

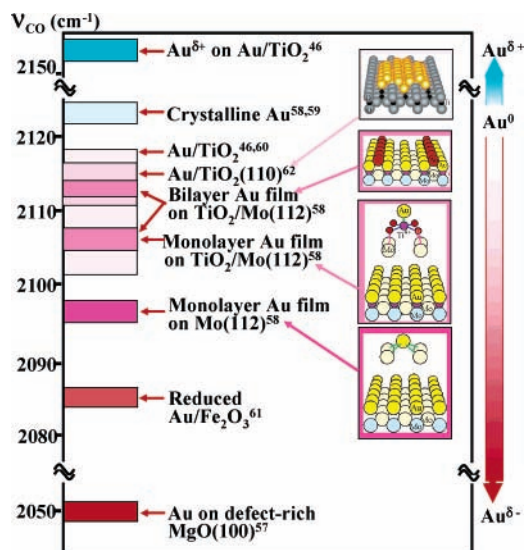


FIGURE 7. Comparison of the stretching frequencies for CO adsorption on various supported Au catalysts.^{46,57–62}

clusters relative to bulk Au and that the extent of the shift can be correlated with the electronic charge on Au.^{46,57,58} The ν_{CO} frequencies for CO adsorption on ordered Au monolayer and bilayer structures are compared with monolayer and multilayer Au on Mo single crystals, together with pertinent literature data, in Figure 7. Note that the surface arrangements of the atoms in monolayer Au on a single crystal Mo surface and monolayer Au on a reduced titania surface are similar, with the exception that, in the former, Au binds directly to the substrate Mo while, in the latter, Au binds to the substrate via Ti. Note also that for monolayer Au on Mo, the extent of the electron transfer from the substrate Mo to Au can be approximated as ~0.08 electrons based on the charge transfer reported for Au/Mo(110).⁶³ For monolayer Au on reduced titania, a single ν_{CO} mode corresponding to CO adsorbed on an atop Au atom is observed at ~2107 cm⁻¹ for low CO exposures. On the bilayer Au on reduced titania, both the first and second layer Au atoms are accessible to CO; thus a broad ν_{CO} feature at 2109 cm⁻¹ is observed, a feature that can be decomposed into two bands at 2107 and 2112 cm⁻¹. These two features correspond to atop adsorbed CO on first layer Au and to CO adsorbed on second layer Au, respectively. These results suggest that CO binds more tightly to first layer than to second layer Au atoms. For CO adsorbed on multilayer Au, for example, 8 monolayers of Au on single-crystal Mo, the ν_{CO} mode is found at 2124 cm⁻¹, a frequency identical to those found for CO on single-crystal Au surfaces.⁵⁹ On a negatively charged Au film,⁶³ that is, monolayer Au on Mo, the ν_{CO} mode is found at 2095 cm⁻¹. As displayed in Figure 7, the ν_{CO} frequencies occur at ~2124, 2112, 2107, and 2095 cm⁻¹ for low CO exposures on multilayer Au on Mo, the second layer of Au in a Au bilayer on titania, monolayer Au on titania, and monolayer Au on Mo, respectively. These observed ν_{CO} frequencies demonstrate that the Au films on reduced titania are electron-rich, for example, Au^{δ-}, and that the extent of electron transfer from the substrate to the Au is less than that for monolayer Au on Mo. This sequence of

ν_{CO} frequencies, or the extent of the electron-rich charge state of Au, is consistent with the order of the heats of adsorption for CO being monolayer Au on Mo > monolayer Au on titania > multilayer or bulk-like Au.⁵⁸

The electron-rich nature of Au nanoparticles is supported by theoretical calculations^{30,45} and ancillary experimental data.^{2,31,64,65} Electron transfer to Au nanoparticles has been probed by laser excitation of TiO₂ nanoparticles coated with Au nanoparticles,⁶⁶ by photoemission spectroscopy (PES), and by STM.⁶⁷ As shown in Figure 7, ν_{CO} frequencies are reported at 2120–2100 cm⁻¹ for CO on Au particles supported on TiO₂,^{45,60} ~2088 cm⁻¹ for Au on Fe₂O₃ (reduced FeO),⁶¹ and 2050 cm⁻¹ on very small Au particles supported on defect-rich MgO.⁵⁷ Electron-rich Au nanoparticles are reported to adsorb O₂ more strongly and to activate the O–O bond via charge transfer from Au by forming a superoxo-like species⁴⁸ and also to facilitate activation of CO.^{19,30,45,68} Furthermore molecularly chemisorbed oxygen on Au/TiO₂ is found to be stable at the surface^{48,51} and to react directly with CO to form CO₂ without O₂ dissociation.⁵² This is consistent with electron-rich Au playing a critical role in O–O bond activation and the reaction pathway for CO oxidation on small Au particles proceeding via a di-oxygen species rather than atomic oxygen. A direct correlation has been found between the activity of Au particles for the catalytic oxidation of CO and the concentration of F-centers (defects) at the surface of a MgO support, implying a critical role of surface F-centers in the activation of Au in Au/MgO catalysts.⁶⁴

Quantum Size Effects. The size of Au nanoparticles has been shown to affect the electronic properties decisively.^{2,18,69} A pronounced energy gap has been revealed by PES and DFT for a 20-atom Au cluster with a tetrahedral structure and atomic packing similar to that of bulk gold.⁷⁰ A metal-to-insulator transition is observed as the size of Au nanoparticles decreases below 3 nm by measuring the tunneling current as a function of the bias voltage ($I - V$)² and by measuring the local barrier height (LBH).⁶⁹ This behavior has also been observed for Pd/TiO₂-(110),²⁵ for Ag particles grown in nanopits on a graphite surface,⁷¹ and for Ag particles supported on Al₂O₃/NiAl-(110).⁷² The valence band structures of (1 × 1) monolayer and (1 × 3) bilayer Au films on reduced titania are significantly different from those of bulk Au,⁵⁸ for example, the electronic properties of the ordered Au films being quite different compared with bulk gold. These size dependences of the electronic and catalytic properties suggest that the pronounced structure sensitivity of CO oxidation on Au/TiO₂ relates to limited size or quantum size effects.

Quantum size effects have been invoked to account for the unique properties of nanometer-scale metallic particles relative to the bulk.^{73–76} Ligand-stabilized metal nanoclusters in the size range of 1–2 nanometers were found to exhibit well-pronounced quantum size behavior.⁷⁷ Ag nanoparticles have been shown theoretically to exhibit three novel, size-dependent vibrational features compared with the bulk⁷⁸ and experimentally to reveal a

series of equidistant resonances near the Fermi level with a decreasing energy separation with increasing cluster size.⁷² Au nanoparticles less than 4 nm were found to exhibit significant quantum size effects with respect to the electronic configuration and the vibrational modes using Au-197 Mossbauer spectroscopy.⁷⁹

Quantum-size effects have also been found to influence the thermodynamic properties of metallic nanoparticles,⁸⁰ properties of superconductors,⁸¹ and chemisorptive properties of nanosized materials.^{19,30,45,63,82–85} Charge transfer for CO adsorption depends critically on the size of a Na quantum dot.⁸⁴ Particle size effects were found for CO adsorption on Au deposits supported on FeO(111) grown on Pt(111)⁸³ and for CO⁶² and oxygen⁸² on Au/TiO₂. Pronounced thickness-dependent variations in the oxidation rate induced by quantum-well states were observed for ordered films up to 15 atomic layers in thickness.⁸⁶ All these studies indicate significant quantum size effects on the electronic, chemical, and catalytic properties of metal nanoparticles.

6. Concluding Remarks

These studies show that ultrathin Au films on a reduced titania surface exhibit catalytic activity comparable to the most active Au nanoparticles, that is, the thickness of the particle rather than the particle diameter is the critical structural feature with respect to catalytic activity. The wetting of Au on a reduced titania surface to form an active bilayer film (two atomic layers in thickness) increases the active site density by 1–3 orders of magnitude compared with typical high-surface-area supported Au catalysts. A bilayer Au structure has been shown to be a critical feature for catalytically active Au nanoparticles, with low-coordinated Au sites, support-to-particle charge effects, and quantum size effects being contributing factors to the activity. The relative contributions of each of these factors to the special catalytic properties of nanosized Au particles are being assessed in ongoing research around the world.

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