materials

MDPI

Communication

A Rational Design of the Sintering-Resistant Au-CeO_2 Nanoparticles Catalysts for CO Oxidation: The Influence of H_2 Pretreatments

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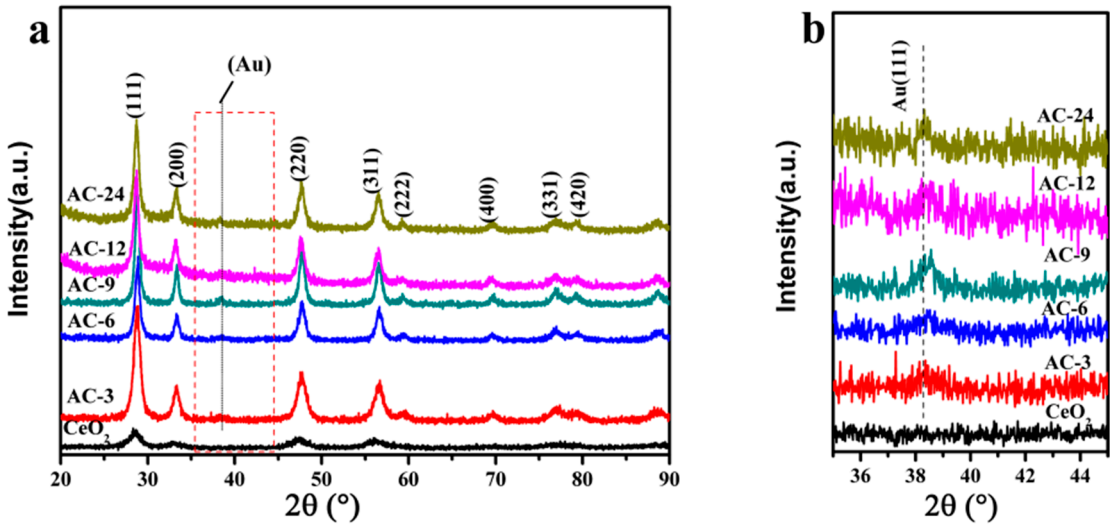

Figure S1. (**a**) X-ray diffraction (XRD) patterns of CeO_2, AC-3, AC-6, AC-9, AC-12 and AC-24 samples; (**b**) the enlargement of the box in (**a**).

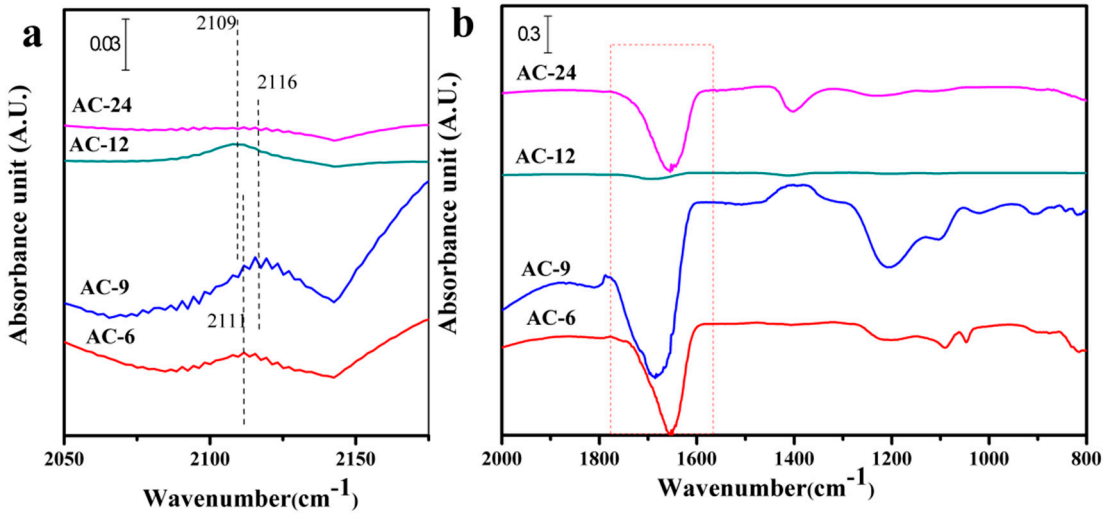

Figure S2. In-situ DRIFT spectra of steady-state CO adsorption after 20 min on Au-CeO_2 samples at RT with the wavenumber region of (**a**) 2200–2050 cm^{-1} bands and (**b**) 2000–800 cm^{-1} bands.

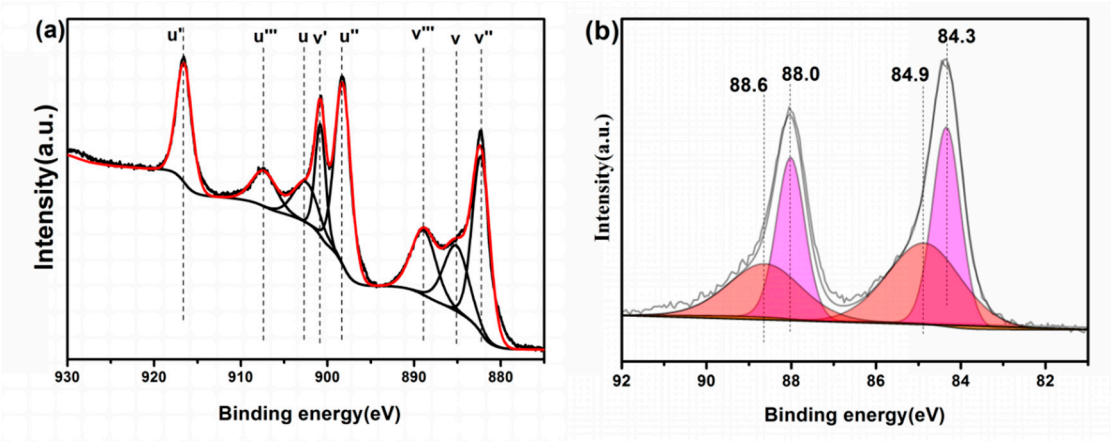

Figure S3. X-ray photoelectron spectra (XPS) of AC-3 (**a**) Ce 3d; (**b**) Au 4f.

Table S1. T_{50} and T_{100} for Au-CeO_2 with or without H_2 pretreatment.

Samples	Unpretreated		H_2 Pretreated	
	T_{50}	T_{90}	T_{50}	T_{90}
AC-3	89	128	46	86
AC-6	70	101	60	106
AC-9	120	188	45	77
AC-12	140	182	46	111
AC-24	159	182	167	192

Table S2. Structural information of the different samples.

sample	CeO_2 Average Crystallite Size (nm)
CeO_2	5.0
AC-3	11.1
AC-6	12.4
AC-9	12.7
AC-12	13.1
AC-24	14.6

Table S3. Structural parameters of Au nanoparticles on various samples.

Samples	Average CeO_2 nanospheres size (nm)	Average Au Nanoparticle Diameter (nm)
AC-3-H	121.8	9.8
AC-6-H	118.4	10.1
AC-9-H	120.2	10.2
AC-12-H	118.5	12
AC-24-H	120.1	13.2

Table S4. Assignment of different types of adsorbed carbonate species.

Species	Wavenumber(cm^{-1})	Wavenumber(cm^{-1}) Pretreatment During CO Absorption					
		AC-3	AC-3-H	AC-6-H	AC-9-H	AC-12-H	AC-24-H
Tridentate carbonates	1048–1073 1266–1276 1460–1550	1051 1269	1051 1269	1051 1269	1051 1269	1051 1269 1515	1269 1500
Bidentate carbonates	1014–1028 ~1319	1319	1319	1023 1319	1023 1319	1319	1319
Bicarbonate species	1600–1616 1618–1638	-	1617	1602	1613	1634	1634

Table S5. Relative content of Ce species for different catalysts obtained from Ce 3d XPS spectra.

Catalysts	Ce^{3+}		Ce^{4+}	
	Peaks	Content (%)	Peaks	Content (%)
AC-3	885.1 902.5	18.4%	882.4, 889.1, 898.3, 900.8, 916.6, 907.4	81.6%
AC-3-H	884.5 901.8	18.3%	881.8, 888.4, 897.7, 900.3, 916.0, 906.8	81.7%
AC-6-H	884.8 902.1	15.1%	882.0, 888.5, 897.9, 900.5, 916.2, 907.1	84.9%
AC-9-H	884.5 902.0	17.5%	881.8, 888.4, 897.8, 900.3, 916.1, 907.0	82.5%
AC-12-H	885.1 902.6	17.2%	882.1, 888.7, 898.0, 900.6, 916.3, 907.1	82.8%
AC-24-H	884.9 902.2	18.6%	881.8, 888.4, 897.8, 900.3, 916.0, 906.9	81.4%

Table S6. Relative content of Au species for different catalysts obtained from Au 4f XPS spectra.

Samples	Au^0			$Au^{\delta+}$		
	Peaks (eV)	content	FWHM (eV)	Peaks	Content	FWHM (eV)
AC-3	84.3 87.8	50.7%	0.78	84.6 88.4	49.3%	2.06
AC-3-H	83.5 87.2	76.8%	0.92	84.2 88.1	23.2%	3.36
AC-6-H	83.7 87.4	71.3%	1.11	84.3 88.5	28.7%	3.36
AC-9-H	83.5 87.2	79.1%	0.89	83.9 87.7	20.9%	2.72
AC-12-H	83.8 87.5	85.2%	1.19	84.6 89.0	14.8%	2.87
AC-24-H	83.5 87.2	78.9%	0.93	83.8 87.5	21.1%	2.3