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Supplementary Material

CO Oxidation at Near-Ambient Temperatures over TiO_2-Supported Pd-Cu Catalysts: Promoting Effect of Pd-Cu Nanointerface and TiO_2 Morphology

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Table S1. Gaussian fit and Peak deconvolution data for Pd 3d XPS in Pd-Cu/TNS.

Model	Gaussian			
Equation	y = y0 + A/(w*sqrt(pi/(4*ln(2)))) * exp(−4*ln(2)*(x-xc)^2/w^2)			
Plot	Peak1(B)	Peak2(B)	Peak3(B)	Peak4(B)
y0	−0.00562 ± 0.0033	−0.00562 ± 0.0033	−0.00562 ± 0.0033	−0.00562 ± 0.0033
xc	336.71876 ± 0.00825	337.99862 ± 0.15579	342.14296 ± 0.01379	343.29934 ± 0.11648
A	1.01823 ± 0.10132	0.74188 ± 0.12277	0.5292 ± 0.02864	1.05198 ± 0.05865
w	1.28561 ± 0.04191	2.44695 ± 0.26283	1.46628 ± 0.04586	5.16122 ± 0.18801
Reduced Chi-Sqr	$1.76019*10^{-4}$			
R-Square (COD)	**0.99655**			
Adj. R-Square	0.99626			

Table S2. Gaussian fit and Peak deconvolution data for Pd 3d XPS in Pd-Cu/TNT.

Model	Gaussian				
Equation	y = y0 + A/(w*sqrt(pi/(4*ln(2)))) * exp(−4*ln(2)*(x-xc)^2/w^2)				
Plot	Peak1(E)	Peak2(E)	Peak3(E)	Peak4(E)	Peak5(E)
y0	0.68289 ± 0.00192	0.68289 ± 0.00192	0.68289 ± 0.00192	0.68289 ± 0.00192	0.68289 ± 0.00192
xc	336.69738 ± 0.01318	338.03611 ± 0.33166	342.12392 ± 0.05905	344.32183 ± 0.1558	346.37533 ± 0.43852
A	0.41585 ± 0.07728	0.31292 ± 0.0873	0.46595 ± 0.03369	0.12966 ± 0.05476	0.06757 ± 0.03534
w	1.44888 ± 0.08567	2.75708 ± 0.46016	2.17613 ± 0.11676	1.94451 ± 0.55714	2.08056 ± 0.66893
Reduced Chi-Sqr	$6.22459*10^{-5}$				
R-Square (COD)	**0.99226**				
Adj. R-Square	0.99141				

Table S3. Gaussian fit and Peak deconvolution data for Pd 3d XPS in Pd-Cu/TNW.

Model	Gaussian				
Equation	y = y0 + A/(w*sqrt(pi/(4*ln(2)))) * exp(−4*ln(2)*(x-xc)^2/w^2)				
Plot	Peak1(C)	Peak2(C)	Peak3(C)	Peak4(C)	Peak5(C)
y0	0.37871 ± 0.00555	0.37871 ± 0.00555	0.37871 ± 0.00555	0.37871 ± 0.00555	0.37871 ± 0.00555
xc	336.60336 ± 0.01681	337.86171 ± 0.23142	341.97893 ± 0.12538	343.61177 ± 0.46675	345.53395 ± 3.48824
A	0.70187 ± 0.09827	0.48683 ± 0.11289	0.62606 ± 0.20328	0.25045 ± 0.56937	0.15445 ± 0.42512
w	1.20458 ± 0.05793	2.26087 ± 0.34057	1.67245 ± 0.1387	2.21717 ± 2.09567	3.11643 ± 3.69335
Reduced Chi-Sqr	$3.36527*10^{-4}$				
R-Square (COD)	**0.9882**				
Adj. R-Square	0.9869				

Table S4. Gauss fit and Peak deconvolution data for O1s XPS in Pd-Cu/TNS.

Model	Gauss	
Equation	y=y0 + (A/(w*sqrt (PI/2)))*exp(−2*((x-xc)/w)^2)	
Plot	Peak1(B)	Peak2(B)
y0	0.00435 ± 0.00211	0.00435 ± 0.00211
xc	529.78156 ± 0.01034	532.31517 ± 0.09681
w	1.36817 ± 0.03138	4.33284 ± 0.15758
A	1.07753 ± 0.03993	1.40001 ± 0.06271
Reduced Chi-Sqr	$4.74279*10^{-4}$	
R-Square(COD)	**0.98608**	
Adj. R-Square	0.98571	

Table S5. Gauss fit and Peak deconvolution data for O1s XPS in Pd-Cu/TNT.

	Gauss			
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(−2*((x-xc)/w)^2)			
Plot	Peak1(B)	Peak2(B)	Peak3(B)	Peak4(B)
y0	$-0.00235 \pm 8.8233*10^{-4}$	$-0.00235 \pm 8.8233*10^{-4}$	$-0.00235 \pm 8.8233*10^{-4}$	$-0.00235 \pm 8.8233*10^{-4}$
xc	529.56114 ± 0.00445	530.91783 ± 0.07997	533.14957 ± 0.53227	542.57941 ± 0.08813
w	1.2495 ± 0.01998	2.32688 ± 0.18827	4.14618 ± 0.47508	5.66583 ± 0.24001
A	0.95349 ± 0.05547	0.82529 ± 0.17062	0.50057 ± 0.13066	0.26406 ± 0.0119
Reduced Chi-Sqr	$2.24717*10^{-5}$			
R-Square(COD)	**0.99935**			
Adj. R-Square	0.99932			

Table S6. Gauss fit and Peak deconvolution data for O1s XPS in Pd-Cu/TNW.

Model	Gauss			
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(−2*((x-xc)/w)^2)			
Plot	Peak1(B)	Peak2(B)	Peak3(B)	Peak4(B)
y0	$-0.00204 \pm 8.56101*10^{-4}$	$-0.00204 \pm 8.56101*10^{-4}$	$-0.00204 \pm 8.56101*10^{-4}$	$-0.00204 \pm 8.56101*10^{-4}$
xc	529.52408 ± 0.0039	530.80478 ± 0.0785	532.9962 ± 0.58344	542.45557 ± 0.09058
w	1.20555 ± 0.01807	2.23169 ± 0.16432	4.10906 ± 0.52062	3.97714 ± 0.22041
A	0.94107 ± 0.05114	0.7681 ± 0.1393	0.3573 ± 0.10215	0.12177 ± 0.00876
Reduced Chi-Sqr	$2.0319*10^{-5}$			
R-Square(COD)	**0.9994**			
Adj. R-Square	0.99937			

Table S7. XPS peak binding energy assignments.

Species /core level	Peak	BE (eV) in Pd-Cu/TNS	BE (eV) in Pd-Cu/TNT	BE (eV) in Pd-Cu/TNW	Oxidation state
Ti 2p	Ti $2p_{3/2}$	458.36	458.26	458.25	
	Ti $2p_{1/2}$	464.23	464.13	464.07	
O 1s		530.1	530	530	
		533.8	532.2	532.5	
Pd 3d	Pd $3d_{5/2}$	337.1	337.1	336.9	Pd^0
	Pd $3d_{3/2}$	342.5	342.5	342.4	
		338.3	338.4	338.3	Pd^{2+}
		343.7	344.7	344	
Cu 2p	Cu $2p_{3/2}$	933.9	932.8	933.2	Cu^{2+} /Cu^{1+}
	Cu $2p_{1/2}$	953.7	952.6	953.2	
	satellite peak	943.3	942.8	943.1	
	satellite peak	962.3	962.1	962.7	

Table S8. CO oxidation activity of our catalysts and other related catalysts.

Catalyst	Synthesis method	T100 (°C)	T50 (°C)	Composition of the feed mixture	Space velocity $mL^{-1}\ g^{-1}\ h^{-1}$)	Reference
Pd/TiO_2-CeO_2	impregnation method	~175 (T80 = 138)	~80	0.45% CO/10% O_2/ N_2	GHSV = 480 000 hr^{-1}	[1]
Pd-Cu/Al_2O_3	impregnation method	140	132	2.5% CO and 20% O_2 in N_2 balance	GHSV = 36,000 hr^{-1}	[2]
Pd/Al_2O_3	impregnation method	260	180	2.5% CO and 20% O_2 in N_2 balance	GHSV = 36,000 hr^{-1}	[2]
Cu/Al_2O_3	impregnation method	280	150	2.5% CO and 20% O_2 in N_2 balance	GHSV = 36,000 hr^{-1}	[2]
50CuO-TiO_2 NT	impregnation method	155	-	4% CO and 20% O_2 in a He balance	72,000	[3]
Pd nanoparticle	hydrothermal reduction	180	-	1.0% CO, 4.0% O_2 in He balance	60,000	[4]
$Co_{0.24}$ $Pd_{0.76}$ bimetallic	hydrothermal co-reduction	110	-	1.0% CO, 4.0% O_2 in He balance	60,000	[4]
Cu/Pd/Al_2O_3	deposition–precipitation and impregnation	~224.9	~124.9	2%CO + 1% O_2+ 97% He	46 700	[5]
Pt–Cu/Nb_2O_5	incipient wetness technique	-	150	30% H_2; 1%CO; 1% O_2 ; 20%CO_2; 10% H_2O; He balance	-	[6]
Pt–Cu/Al_2O_3	incipient wetness technique	-	350	30% H_2; 1%CO; 1% O_2; 20%CO_2; 10% H_2O; He balance	-	[6]
20%Cu/Al_2O_3	impregnation method	~540	~420	1600 ppm CO, 1.9% O2 in He	-	[7]
2Ce–20Cu/Al_2O_3	impregnation method	440	~250	1600 ppm CO, 1.9% O2 in He	-	[7]
10.5La_2O_3–20CuO/Al_2O_3	impregnation method		250	1600 ppm CO, 1.9% O_2 in He	-	[7]
graphene-PdPt alloy nanoparticles	wet-chemical route	158 (nanoflower)	-	CO (0.982%) and O_2 (0.493%) in H_2 flow at	GHSV = 47746 hr^{-1}	[8]
		75 (urchin)	-			
Ce-La-20Cu-O	microwave radiation coupled with sol-gel method	225	160	4% CO, 20% O_2 and balance He	60,000	[9]
Pt, Pd, Ir, Rh and Au) supported on TiO_2	liquid phase reduction deposition	165 (Au=Pt) > Pd > Rh > Ir 290	-	5% CO, 10% O_2 in He	-	[10]
Pd supported on (CeO_2 ,TiO_2 ,Al_2O_3 ,ZrO_2 and SiO_2	impregnation method	150 in Pd/CeO_2 < Pd/TiO_2 < Pd/Al_2O_3 < Pd/ZrO_2 ≤ Pd/SiO_2	97 Pd/CeO and 168 in Pd/SiO_2	0.45% CO/10% O_2/He	GHSV = 480,000 hr^{-1}	[11]

Pd_{48}-Cu_{52}/Ce_2O_3	wet chemical synthesis	-	~110	0.5 vol % CO + 10 vol % O_2balanced by N_2	GHSV = 16,000 hr^{-1}	[12]
Pd_{48}-Cu_{52}/TiO_2	wet chemical synthesis	-	70	0.5 vol % CO + 10 vol % O_2balanced by N_2	GHSV = 16,000 hr^{-1}	[12]
Pd/(Ni,Co,Cu)/HNTs	impregnation method	119–146	122–164	4 vol% CO, 20 vol% O_2	72,000	[13]
AuCu/TiO_2	solvothermal	125	80	1 vol% CO, 5 vol% O_2	20000	[14]
CuO/TiO_2	co-precipitation	120	76	1% CO + 5% O_2 (balance N_2)	60 000	[15]
CuO/TiO_2	impregnation	T90=188	-	1% CO + 5% O_2 (balance N_2)	60 000	[15]
CuO-NPs/50-facet Cu_2O	thermal using ascorbic acid as a reducing agen	~175		% $O_2$and 4% CO in He	-	[16]
Cu-TNS	wet impregnation	225.8	144.1	4%CO and 20% O_2 (with Ar as balance	72,000	
Cu-TNT	wet impregnation	205.1	126.2	4%CO and 20% O_2 (with Ar as balance	72,000	
Cu-TNW	wet impregnation	148.7	103.3	4%CO and 20% O_2 (with Ar as balance	72,000	
Pd-TNS	wet impregnation	95.4	92.7	4%CO and 20% O_2 (with Ar as balance	72,000	
Pd-TNT	wet impregnation	78.9	75.7	4%CO and 20% O_2 (with Ar as balance	72,000	This work
Pd-TNW	wet impregnation	69.5	67.2	4%CO and 20% O_2 (with Ar as balance	72,000	
Pd-Cu/TNS	wet impregnation	67.2	64.6	4%CO and 20% O_2 (with Ar as balance	72,000	
Pd-Cu/TNT	wet impregnation	57.4	53.5	4%CO and 20% O_2 (with Ar as balance	72,000	
Pd-Cu/TNW	wet impregnation	43.8	41.92	4%CO and 20% O_2 (with Ar as balance	72,000	
(Cu, Co, Mn, Fe, Ni, Zr, and Zn)/CeO_2	microwave assisted sol−gel synthesis	~575(Zn) – 75 (Cu)	~(275) Zn> Fe> Mn> Ni> Co> Cu (63)	4 vol% CO, 20 vol% O_2 (He as balance gas)	60,000	[17]

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