

**Supporting Information for**

**Towards quantitative and scalable transformation of furfural to cyclopentanone  
with supported gold catalysts**

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**Table S1.** Effect of additives on the transformation of furfural (FFA) over 0.73 wt% Au/TiO<sub>2</sub>-A.<sup>[a]</sup>

Entry	Additive	Conv. [%]	Mass balance [%]	Sel. [%]				
				CPO	CPL	MF	FAL	CEON
1	Na <sub>2</sub> CO <sub>3</sub>	>99	27±5	0	0	3	24	0
2	Na <sub>2</sub> HPO <sub>4</sub>	>99	48±3	0	0	7	41	0
3	none	>99	99±1	>99	0	0	0	0
4	NaH <sub>2</sub> PO <sub>4</sub>	>99	64±3	47	1	0	11	5
5	H <sub>3</sub> PO <sub>4</sub>	>99	31±5	19	2	0	4	6

[a] Reaction conditions: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), additive (0.1 mmol), H<sub>2</sub> (4 MPa), S/C (2000), 160 °C, 1.2 h.

**Table S2.** The hydrogenation of FFA over platinum-group-metal (PGM)-based catalysts.<sup>[a]</sup>

Entry	catalyst <sup>[b]</sup>	Conv. [%]	Mass balance [%]	Sel. [%]				
				CPO	CPL	MF	FAL	CEON
1	Pt/TiO <sub>2</sub> -A (0.73 wt%)	87	87±3	71	5	11	0	0
2	Pd/TiO <sub>2</sub> -A (0.73 wt%)	23	95±2	87	1	6	0	1
3	Ir/TiO <sub>2</sub> -A (0.73 wt%)	56	93±2	34	0	0	0	59
4	Rh/TiO <sub>2</sub> -A (0.73 wt%)	41	94±2	93	0	0	0	1

[a] Reaction conditions: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), H<sub>2</sub> (4 MPa), S/C (2000), 160 °C, 1.2 h.

**Table S3.** The hydrogenation of FFA over TiO<sub>2</sub>-A supported noble catalysts at 80 °C.<sup>[a]</sup>

Entry	catalyst	Conv. [%]	Sel. [%]	
			FAL	other
1	Au/TiO <sub>2</sub> -A (0.73 wt%)	31	99	0
2	Pt/TiO <sub>2</sub> -A (0.73 wt%)	82	99	0
3	Pd/TiO <sub>2</sub> -A (0.73 wt%)	63	99	0

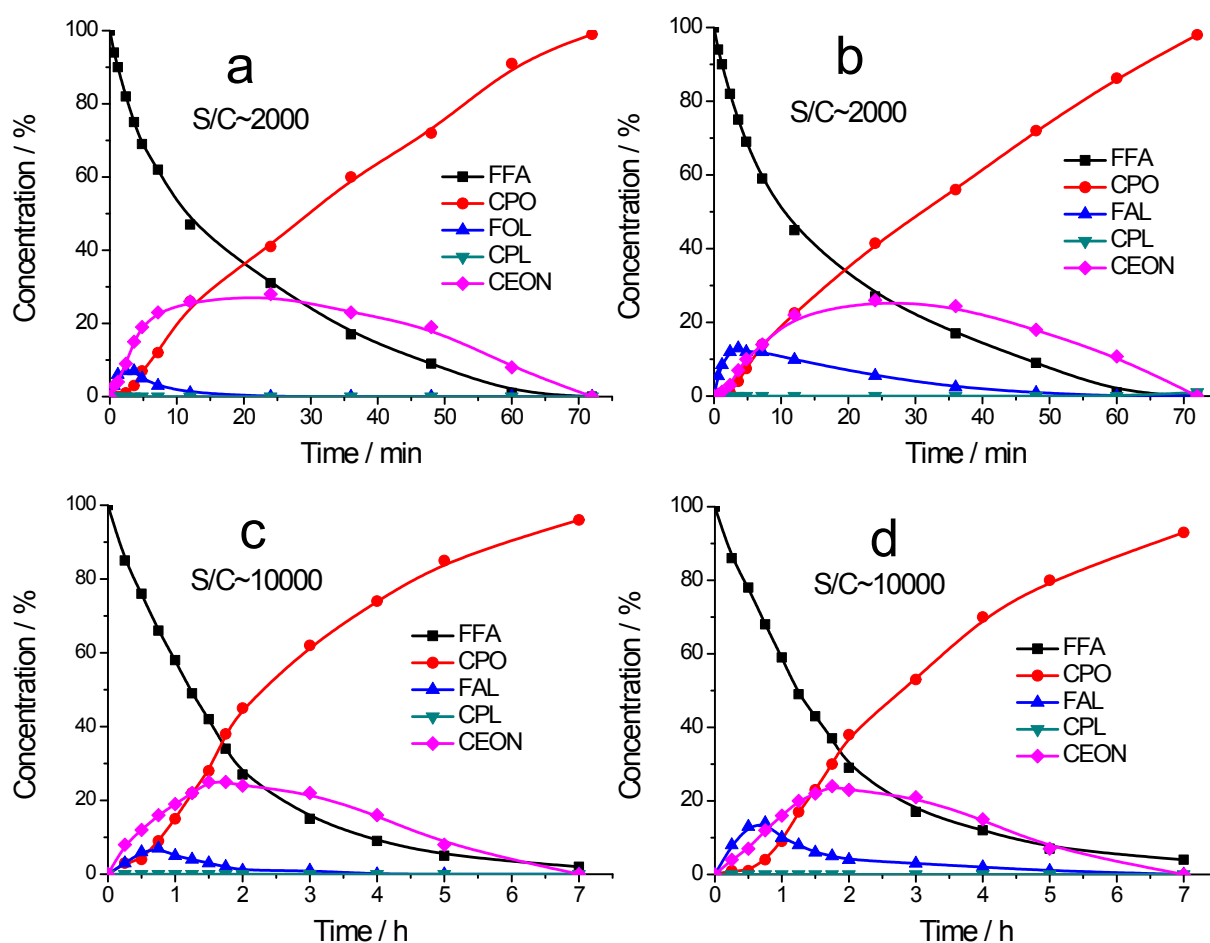
[a] Reaction conditions: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), H<sub>2</sub> (4 MPa), S/C (2000), 80 °C, 1.2 h.

**Table S4.** The effect of different-sized gold particles and various gold loadings on the transformation of FFA to CPO.<sup>[a]</sup>

Entry	Catalyst	Average particle size [nm]	Conv. [%]	TOF <sup>[b]</sup> [h <sup>-1</sup> ]	Mass balance [%]	Sel. [%]			
						CPO	CPL	FAL	CEON

1	Au/TiO <sub>2</sub> -A (0.73wt%)	2.1	>99	7520	99±1	>99	0	0	0
2	Au/TiO <sub>2</sub> -A (0.71wt%)	4.6 <sup>[c]</sup>	35	680	99±1	36	0	25	38
3	Au/TiO <sub>2</sub> -A (0.75wt%)	8.4 <sup>[d]</sup>	16	270	99±1	25	0	28	46
4	Au/TiO <sub>2</sub> -A (0.24wt%)	2.1	>99	7560	99±1	>99	0	0	0
5	Au/TiO <sub>2</sub> -A (0.10wt%)	2.0	>99	7470	99±1	>99	0	0	0

[a] Reaction conditions: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), H<sub>2</sub> (4 MPa), S/C (2000), 160 °C, 1.2 h; [b] TOF values based on total the gold loading at FFA conversion of 15%; [c] Figure S9e; [d] Figure S9f.

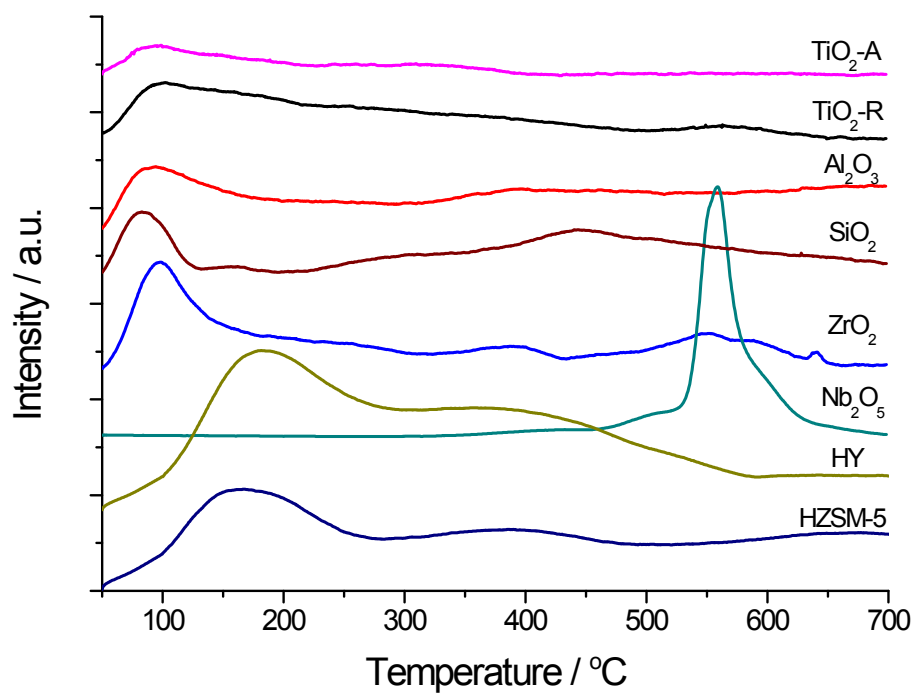


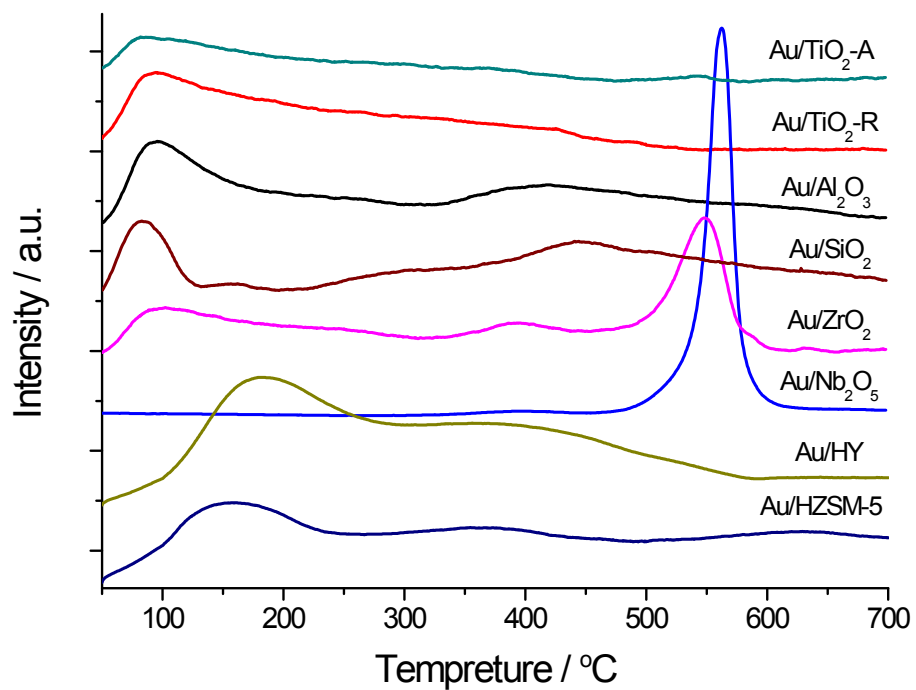
**Figure S1.** Reaction profiles for the hydrogenation of FFA over a series of Au/TiO<sub>2</sub>-A catalysts with different gold loading content or S/C levels. (a) 0.24 wt% Au/TiO<sub>2</sub>-A (S/C~2000); (b) 0.73 wt% Au/TiO<sub>2</sub>-A mixed with seven-fold bare TiO<sub>2</sub>-A (S/C~2000); (c) 0.24 wt% Au/TiO<sub>2</sub>-A (S/C~10000); (d) 0.73 wt% Au/TiO<sub>2</sub>-A (S/C~10000). Reaction condition: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), H<sub>2</sub> (4 MPa), 160 °C.

**Table S5.** The effect of reaction temperature and hydrogen pressure on the transformation of FFA to CPO over 0.10 wt% Au/TiO<sub>2</sub>-A.<sup>[a]</sup>

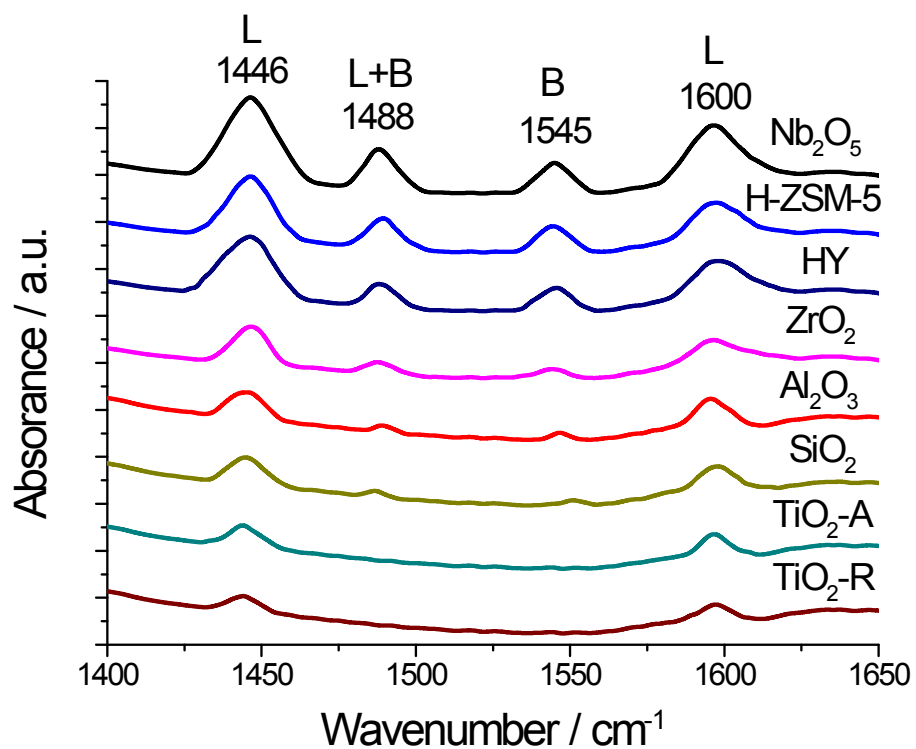
Entry	H <sub>2</sub> [MPa]	T [°C]	Conv. [%]	Mass balance [%]	Sel. [%]			
					CPO	CPL	FAL	CEON
1	4	120	42	99±1	18	0	71	10
2	4	140	77	99±1	76	0	10	13
3	4	160	>99	99±1	>99	0	0	0
4	4	180	>99	95±2	88	7	0	0
5	3	160	92	99±1	86	0	0	13
6	5	160	>99	99±1	96	3	0	0

[a] Reaction conditions: FFA (5.2 mmol), H<sub>2</sub>O (10 mL), S/C (2000), 1.2 h.

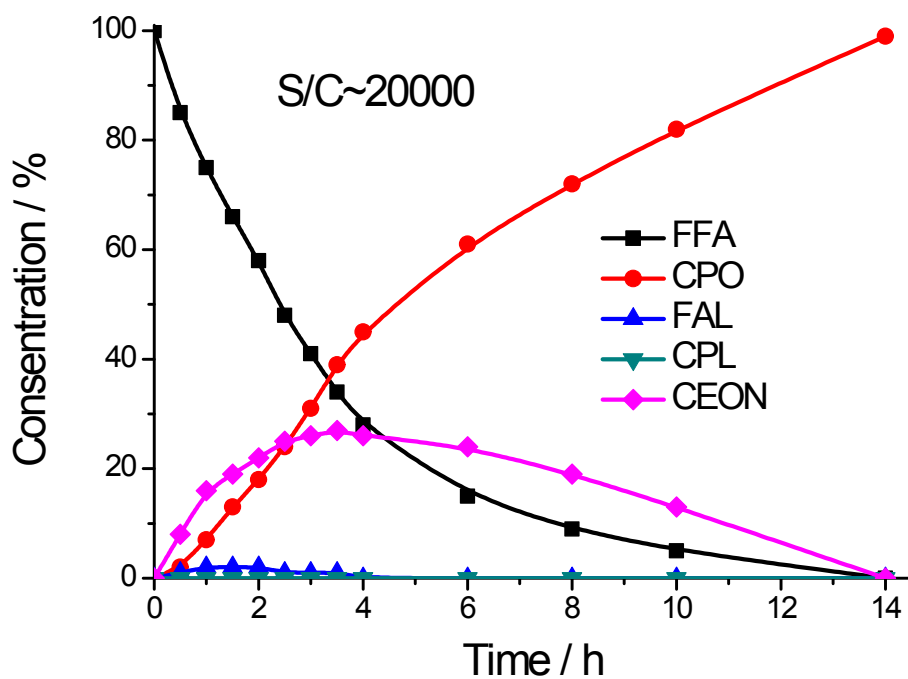




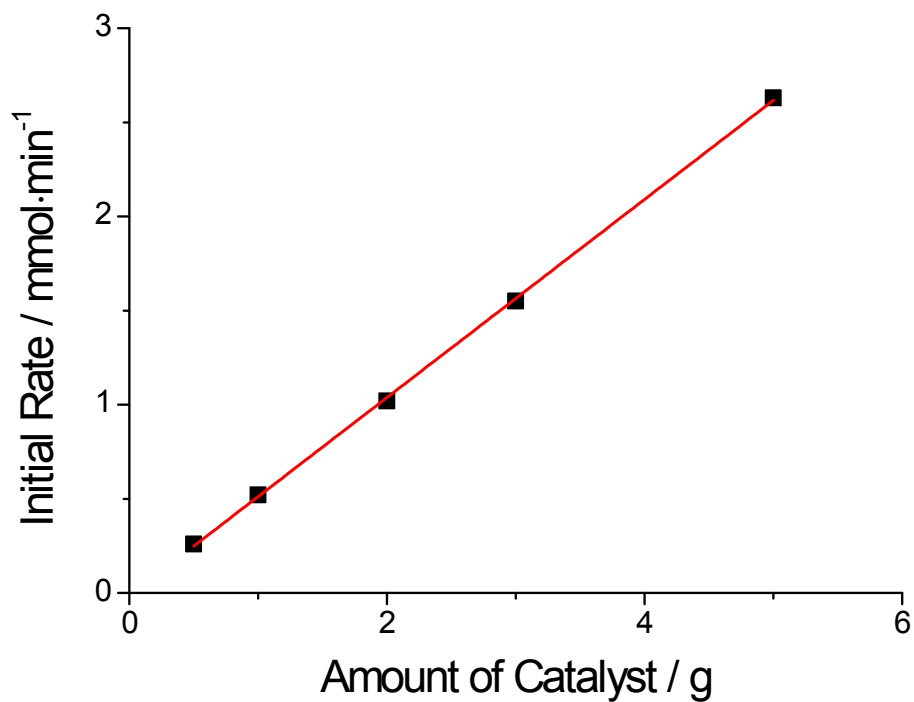
**Figure S2.** NH<sub>3</sub>-TPD profiles of various supports and gold catalysts.



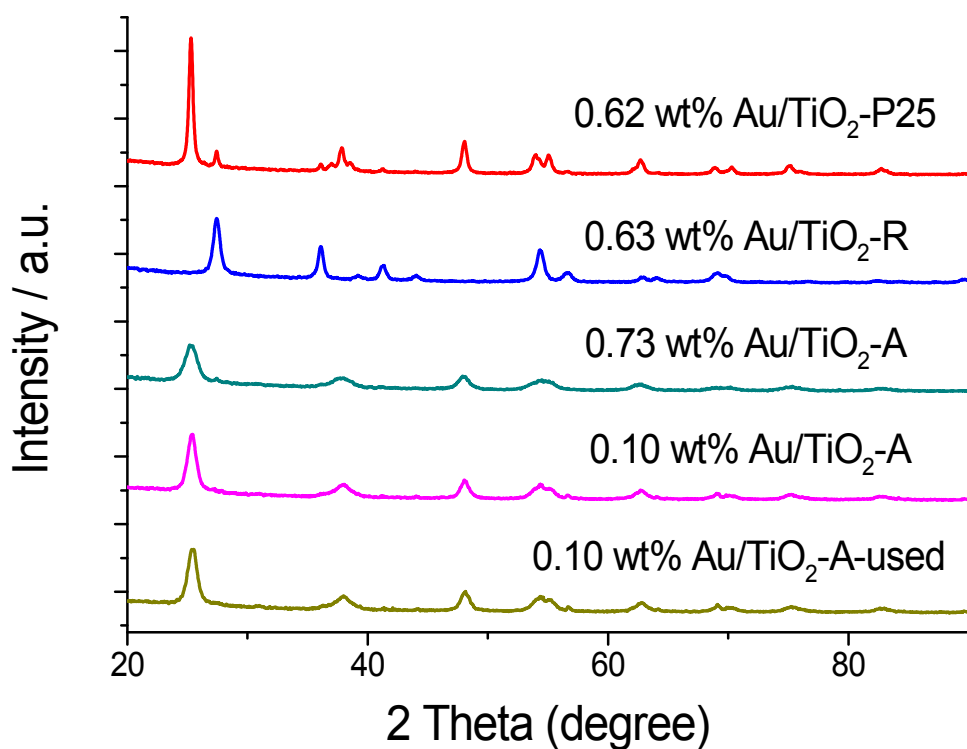
**Figure S3.** FTIR spectra of pyridine adsorbed onto the various oxide supports.



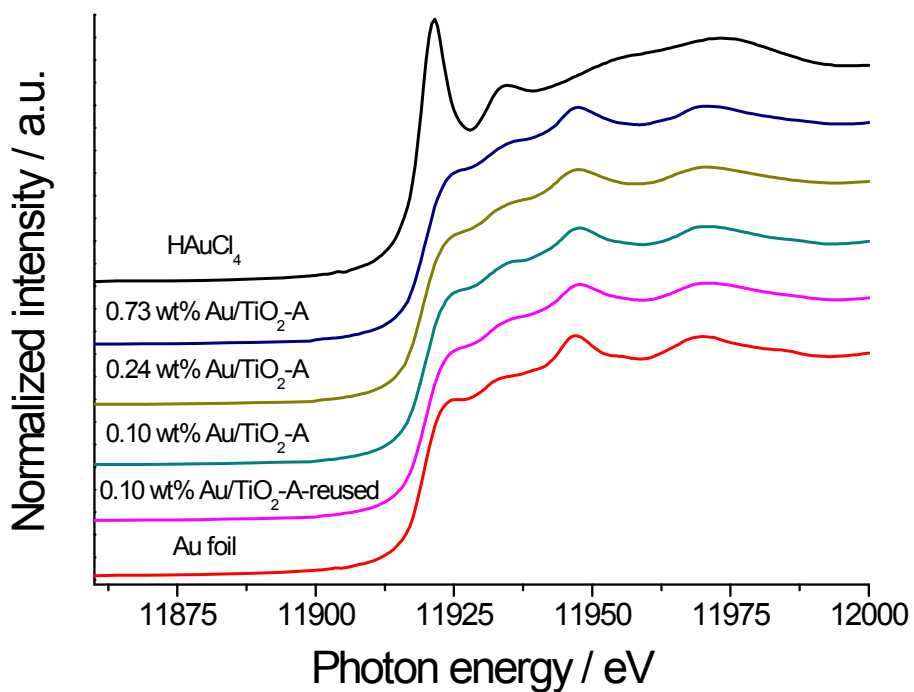
**Figure S4.** Kinetic profiles of 50 mmol scale. Reaction condition: FFA (50 mmol), catalyst (0.10 wt% Au/TiO<sub>2</sub>-A), H<sub>2</sub>O (100 mL), H<sub>2</sub> (4 MPa), S/C (20000), 160 °C.



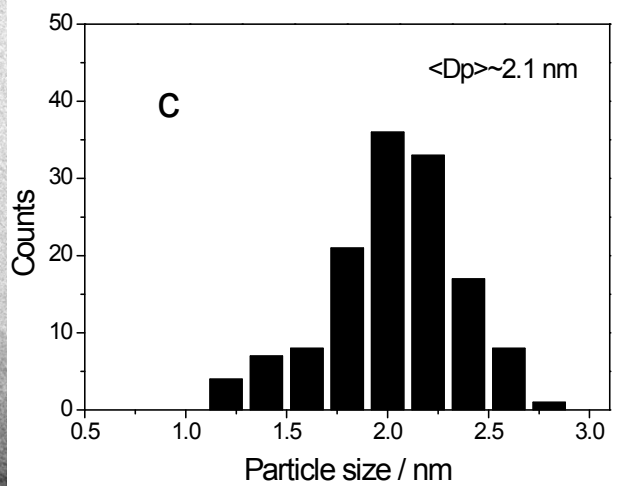
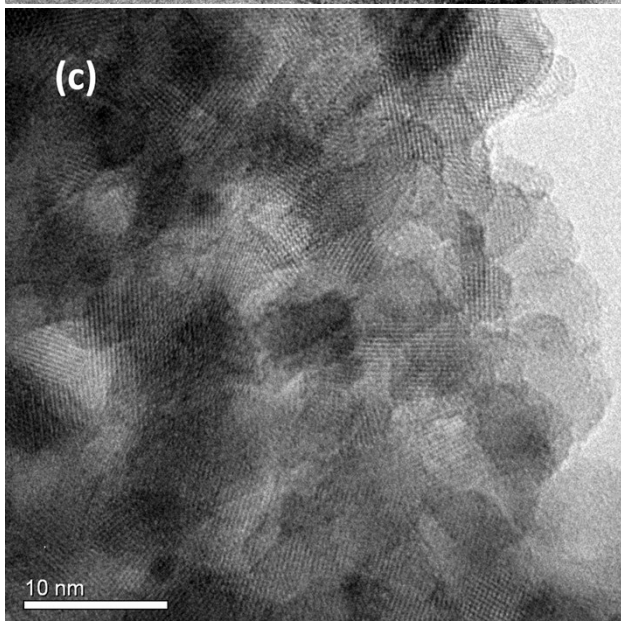
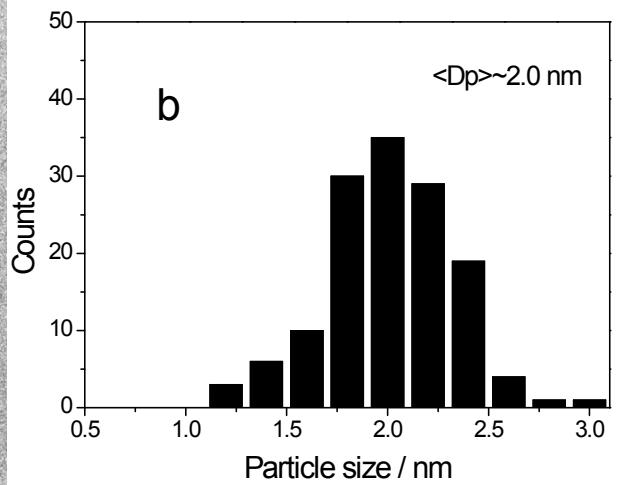
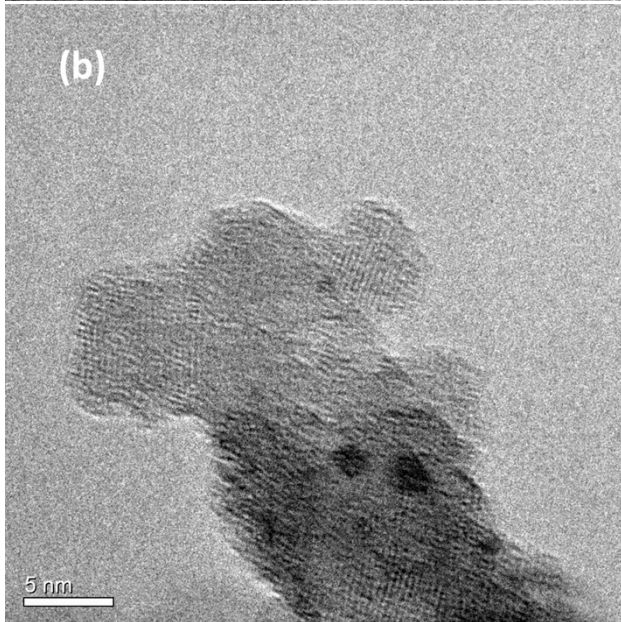
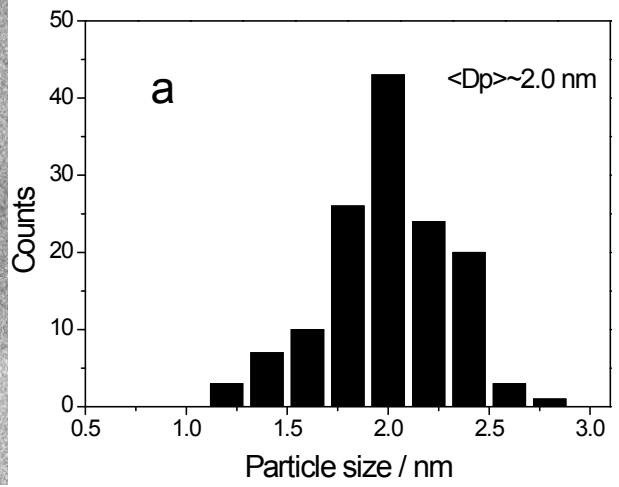
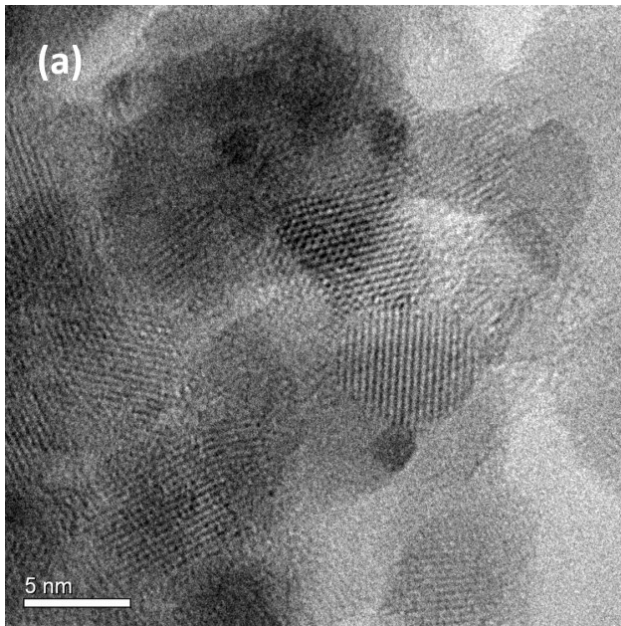
**Figure S5.** Dependence of the initial reaction rates on the catalyst concentration for the transformation of furfural. Reaction condition: FFA (50 mmol), H<sub>2</sub>O (100 mL), H<sub>2</sub> (4 MPa), catalyst (0.10 wt% Au/TiO<sub>2</sub>-A), 160 °C, conversion of FFA (15%).



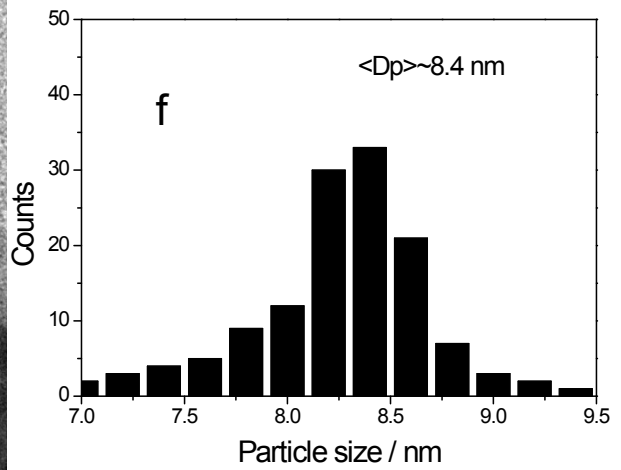
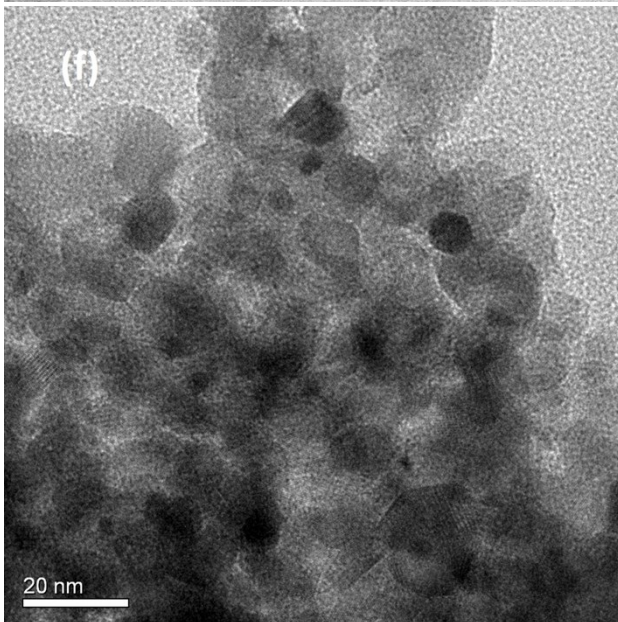
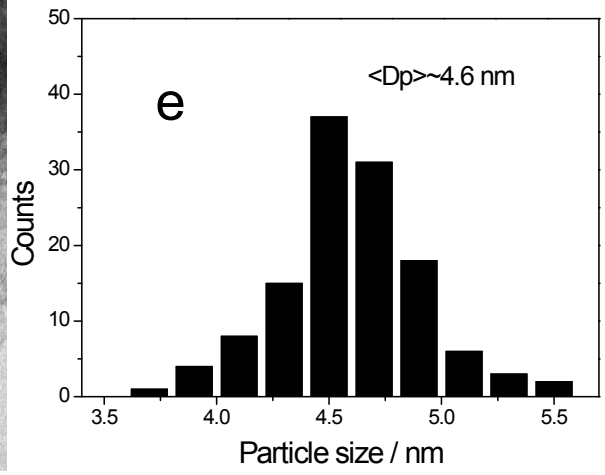
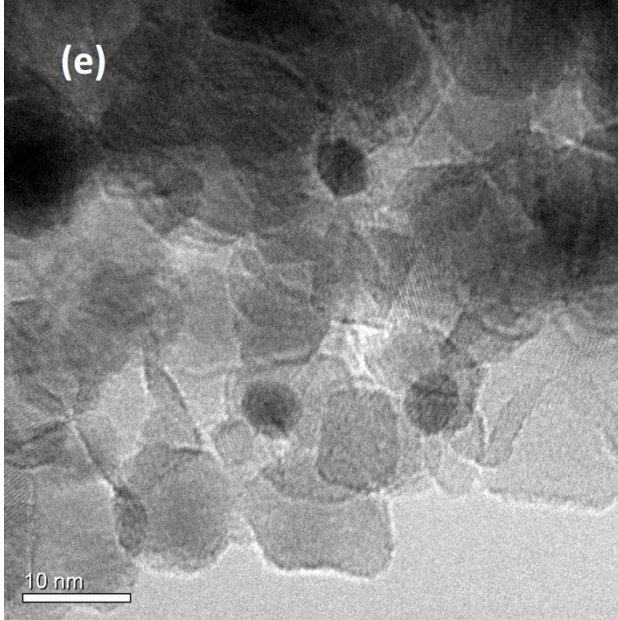
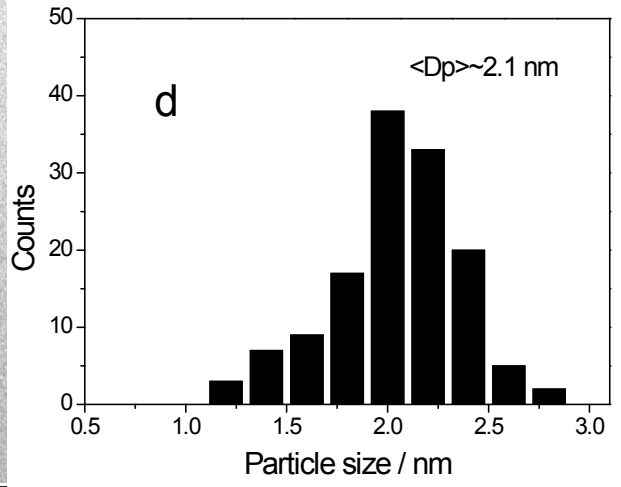
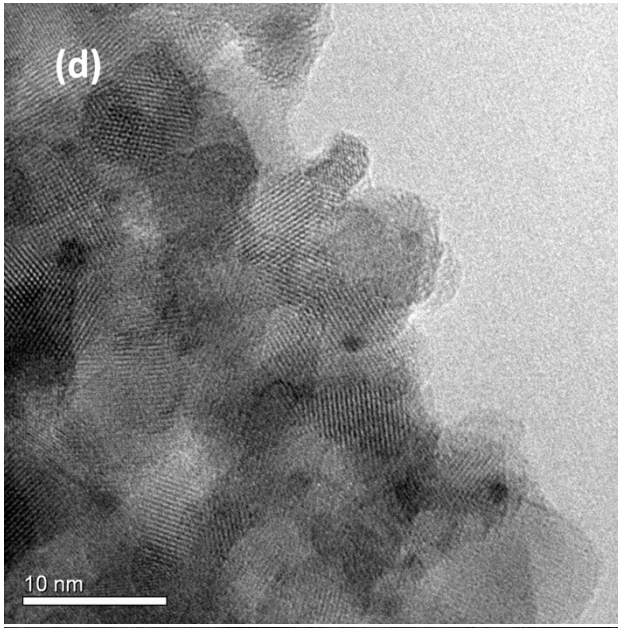
**Figure S6.** Powder XRD patterns of various Au/TiO<sub>2</sub> catalysts.

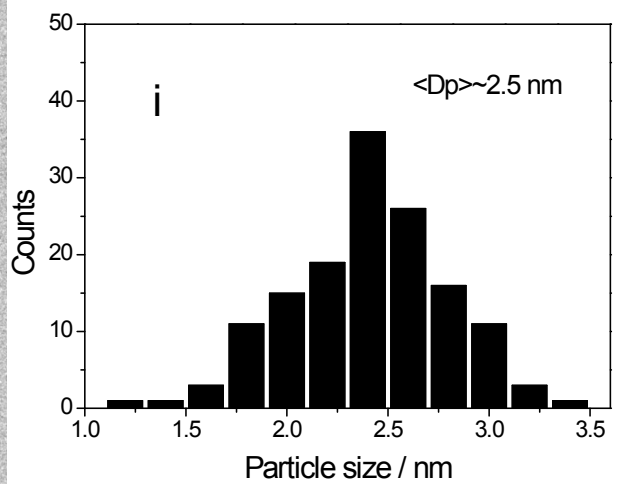
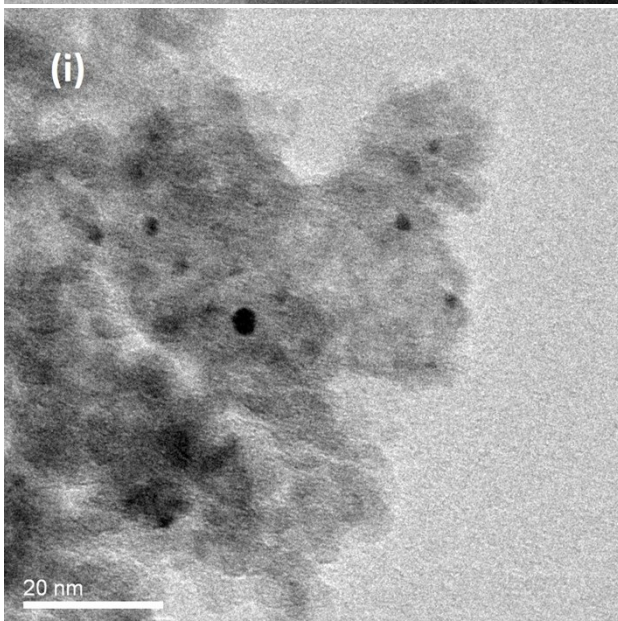
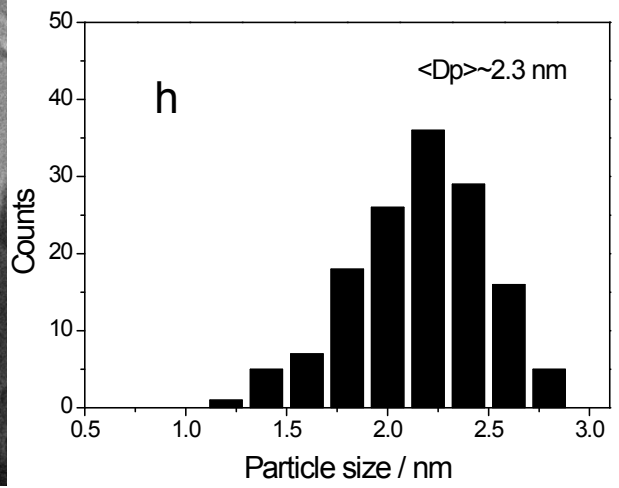
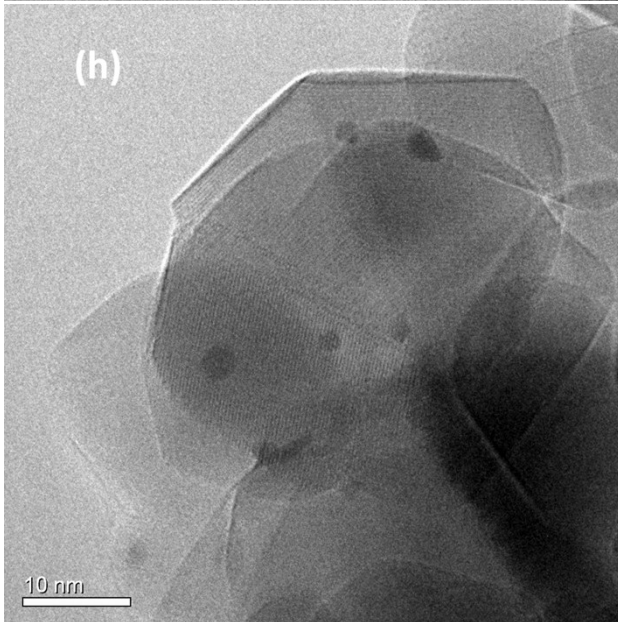
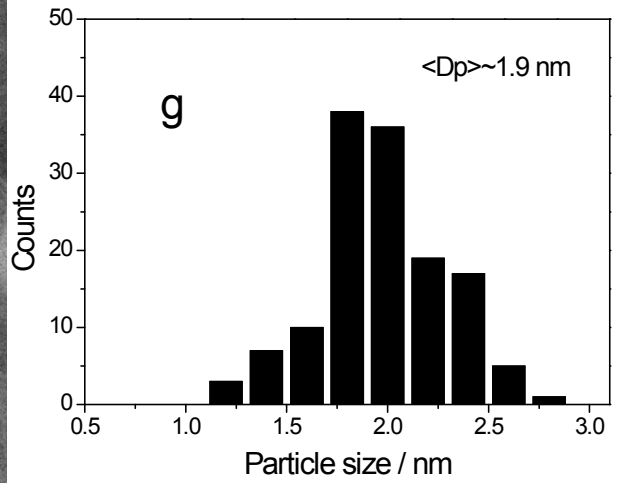
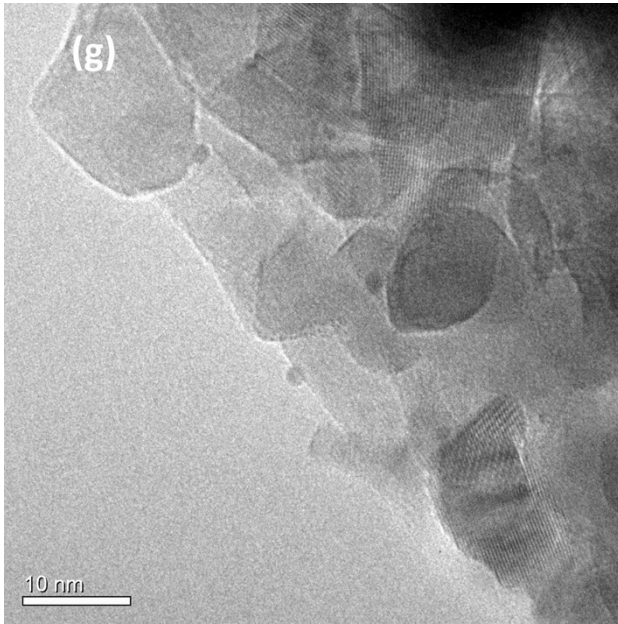


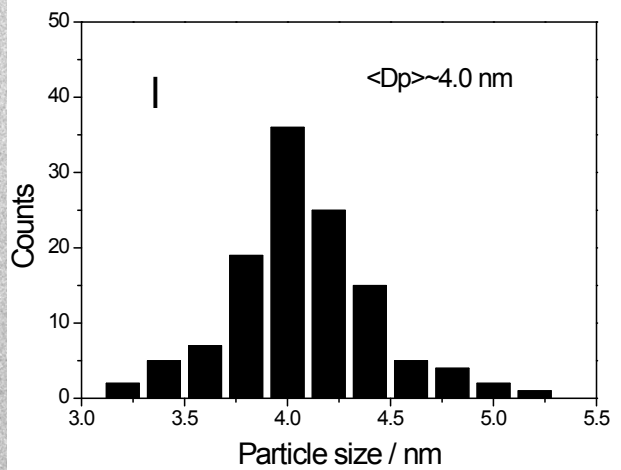
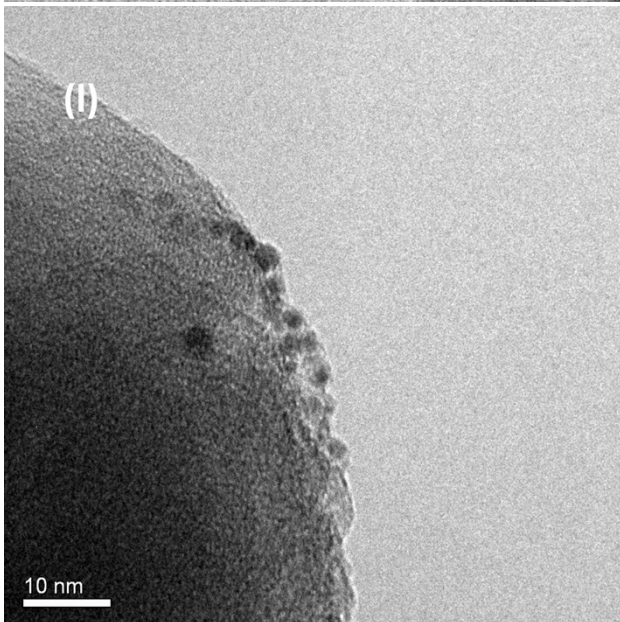
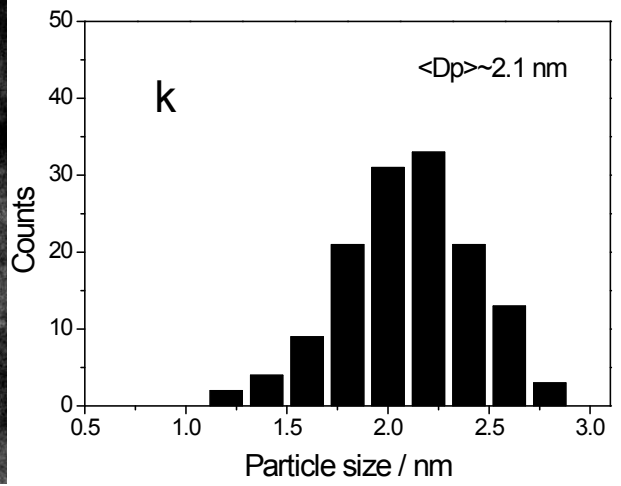
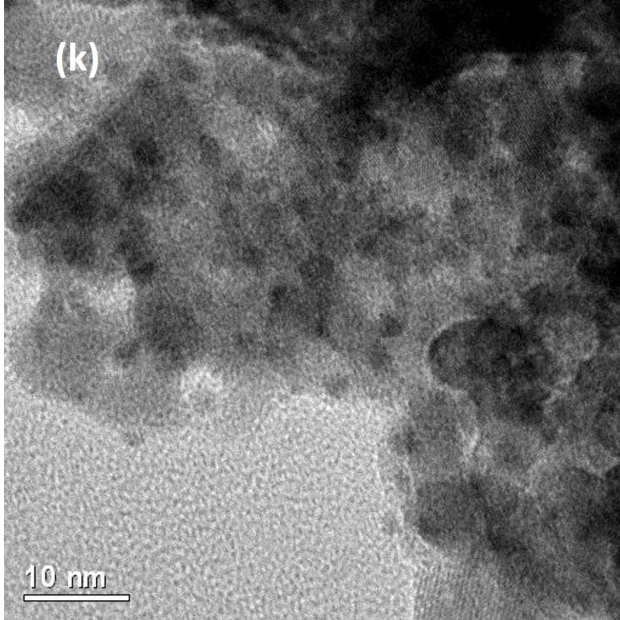
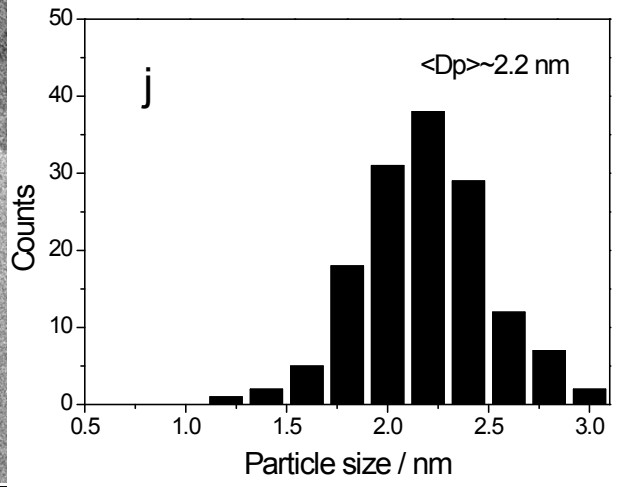
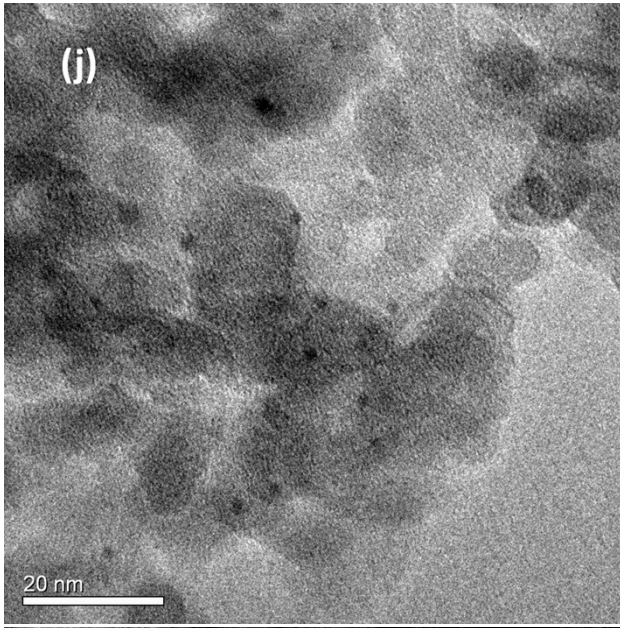
**Figure S7.** XANES analysis of Au/TiO<sub>2</sub>-A catalyst.

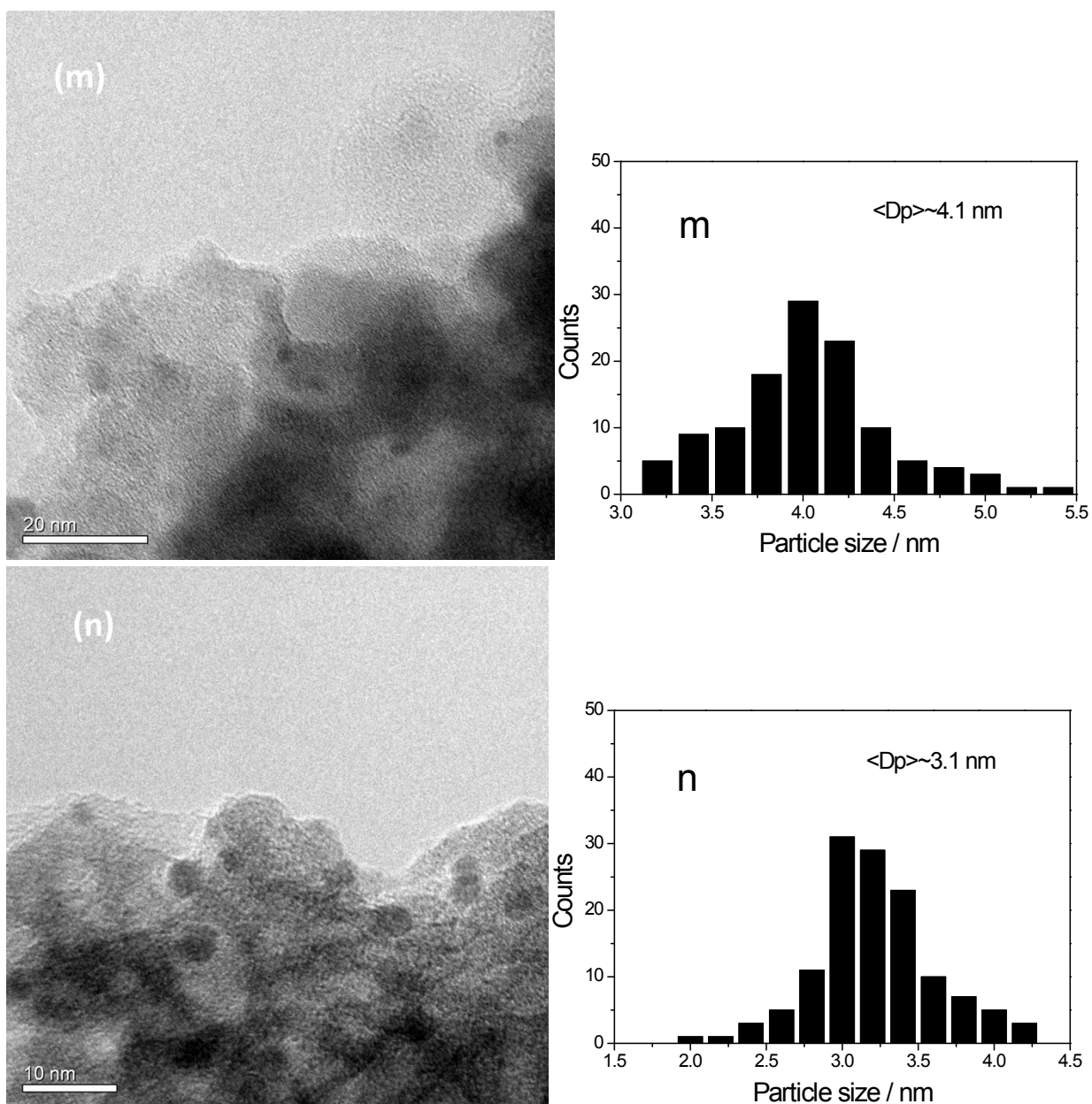




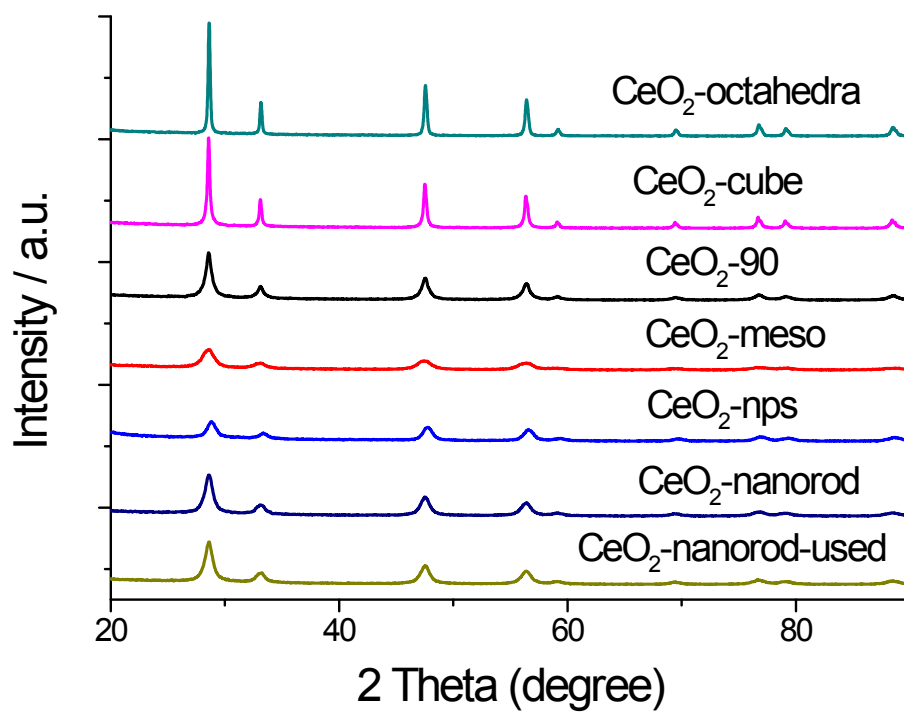




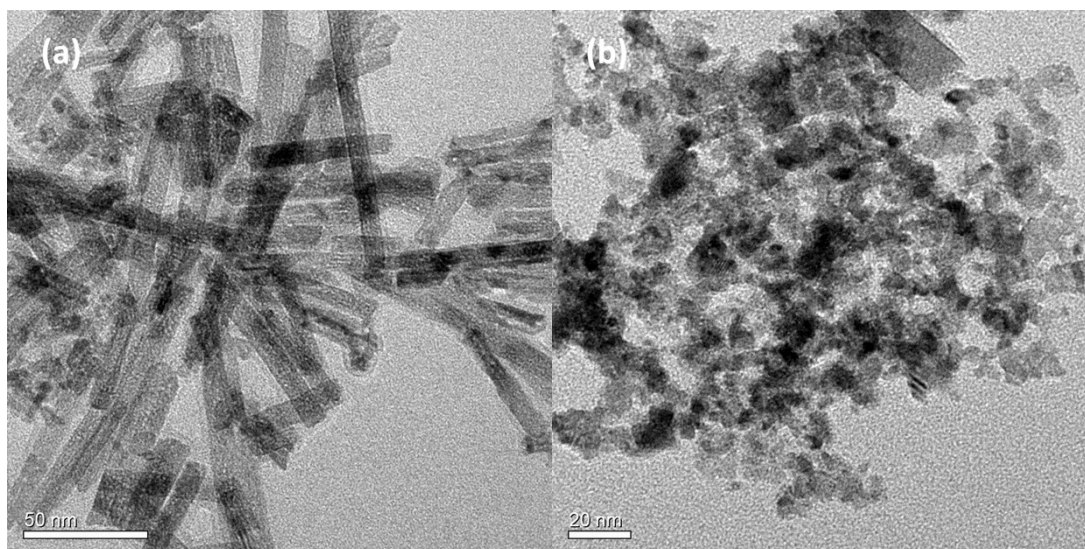


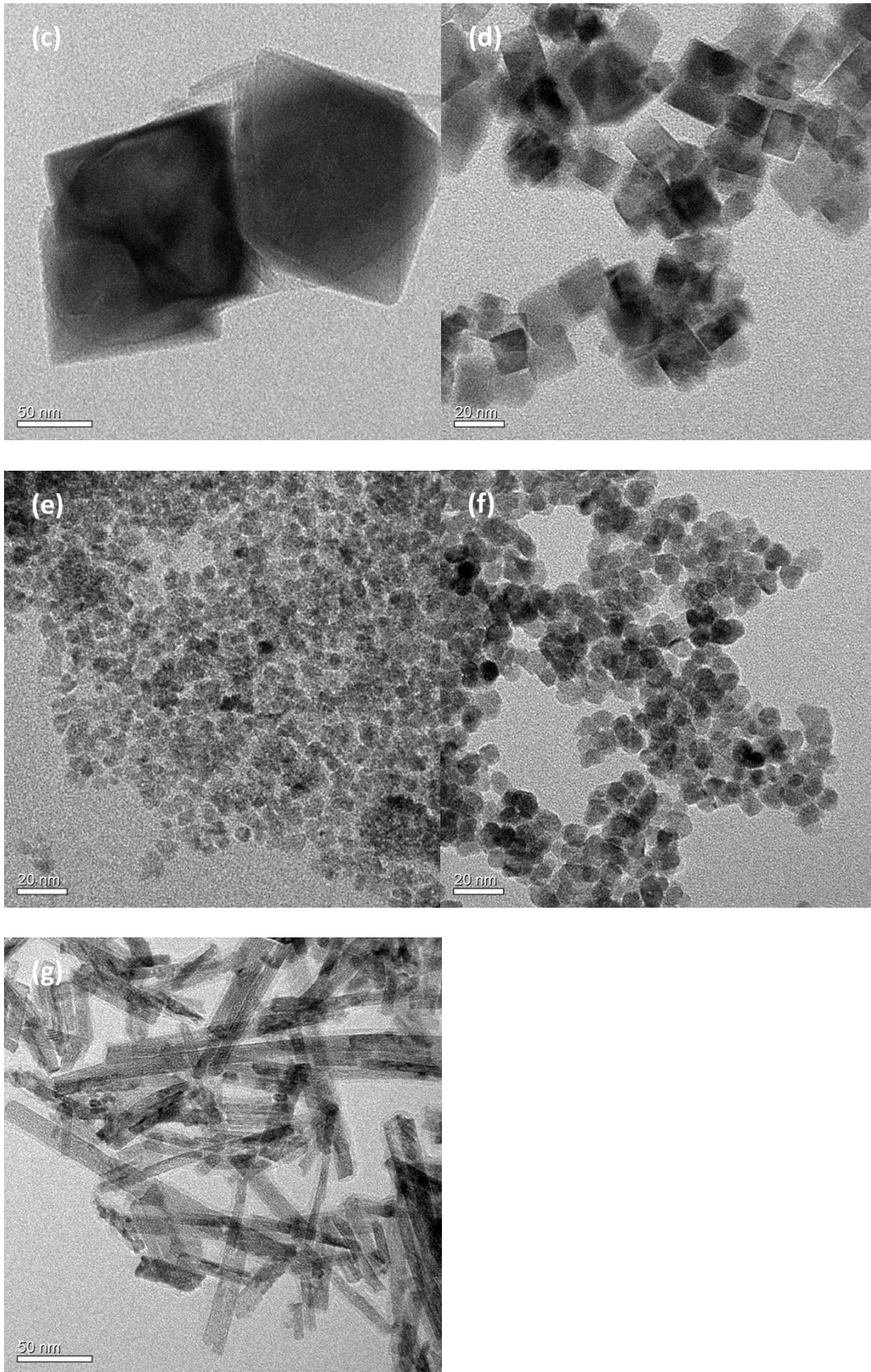


**Figure S8.** TEM analysis of various catalysts (a) 0.10 wt% Au/TiO<sub>2</sub>-A; (b) 0.10 wt% Au/TiO<sub>2</sub>-A-reused; (c) 0.24 wt% Au/TiO<sub>2</sub>-A; (d) 0.73 wt% Au/TiO<sub>2</sub>-A; (e) 0.71 wt% Au/TiO<sub>2</sub>-A (4.6 nm); (f) 0.75 wt% Au/TiO<sub>2</sub>-A (8.4 nm); (g) 0.63 wt% Au/TiO<sub>2</sub>-R; (h) 0.62 wt% Au/TiO<sub>2</sub>-P25; (i) 0.85 wt% Au/Al<sub>2</sub>O<sub>3</sub>; (j) 0.65 wt% Au/SiO<sub>2</sub>; (k) 0.68 wt% Au/ZrO<sub>2</sub>; (l) 0.64 wt% Au/HY; (m) 0.62 wt% Au/H-ZSM-5; (n) 0.61 wt% Au/Nb<sub>2</sub>O<sub>5</sub>.



**Figure S9.** XRD analysis of various forms of nanostructured CeO<sub>2</sub>.





**Figure S10.** TEM analysis of various forms of nanostructured CeO<sub>2</sub>. (a) CeO<sub>2</sub>-nanorods; (b) CeO<sub>2</sub>-90; (c) CeO<sub>2</sub>-octahedra; (d) CeO<sub>2</sub>-cube; (e) CeO<sub>2</sub>-meso; (f) CeO<sub>2</sub>-nps; (g) CeO<sub>2</sub>-nanorods-used.