Electronic Supplementary Material (ESI) for RSC Advances.

Gold Supported on Ti Incorporated MCM-36 as Efficient Catalysts in Propylene Epoxidation with H_2 and O_2

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Supporting information

Table S1. Catalytic performance over different catalysts mAu/*x*Si/Ti-MCM-36 and mAuNH_3/*x*Si/Ti-MCM-36.

Catalyst	Si/Ti atomic ratio	Au wt%	T (K)	PO yield (%)	Propene conv.(%)	Selectivity (%)				CO_2 select. (%)	H_2 conv. (%)	H_2 select. (%)	PO rate ($g*h^{-1}*kg_{ca}^{-1}$)	TOR ($g_{PO}*h^{-1}*g_{Au-1}$)
						PO	PA	ACR	ACE					
4.5Au/*100*Si/Ti-MCM-36	30	0.84	453	(0.9)	(0.88)	(84.93)	(0)	(4.55)	(0)	(10.23)	(19.61)	(3.81)	(13.9)	(1.65)
				0.67	0.71	93.02	0	0.91	0	6.01	14.46	4.68	10.25	1.22
			433	0.51	0.55	94.49	0	1.14	0	4.3	14.79	3.49	7.91	0.94
			473	0.44	0.55	79.43	4.97	3.55	0	11.97	18.81	2.35	6.77	0.81
3Au/1*00*Si/Ti-MCM-36	30	0.36	453	(1.88)	(2.98)	(62.99)	(1.68)	(4.7)	(0.34)	(30.2)	(43.36)	(4.33)	(28.91)	(8.03)
				1.01	1.57	63.08	0	14.68	0	22.25	26.72	4.28	15.49	5.53
			433	0.97	1.2	81.07	0	8.25	0	10.69	28.94	5.53	14.99	5.35
			473	0.98	2.05	48.63	5.17	27.09	0	19.15	38.09	3.92	15.16	5.42
1.5Au/1*00*Si/Ti-MCM-36	30	0.19	453	(1.8)	(2.19)	(82.24)	(1.37)	(0)	(0)	(16.29)	(18.51)	(9.73)	(27.74)	(14.6)
				1.39	1.61	86.61	0.23	0	0	13.14	11.36	12.78	21.43	11.28
			433	1.33	1.49	90.74	0.3	0	0	9.01	8.98	16.74	20.51	10.8
			473	1.1	1.6	67.45	2.6	0.92	0	29.06	17.72	6.17	16.93	8.91
1Au/*100*Si/Ti-MCM-36	30	0.12	453	(0.93)	(1.08)	(86.02)	(0)	(0)	(0)	(13.58)	(16.57)	(5.61)	(14.31)	(11.93)
				0.48	0.61	77.49	0	0	0	22.47	12.58	3.65	7.42	6.18
1.5Au/*40*Si/Ti-MCM-36	15.3	0.31	453	(1.31)	(2.12)	(61.83)	(5.19)	(2．83)	(0)	(30.19)	(33.78)	(3.88)	(19．41)	(16.18)
				0.39	0.65	62.9	9.18	0.57	0	27.34	19.18	1.86	5.79	4.82
1.5Au/*160*Ti-MCM-36	94	0.14	453	(0.97)	(2.22)	(43.58)	(18.47)	(0)	(0)	(38.14)	(28.32)	(3.42)	(14.9)	(4.81)
				0.39	0.97	41.39	5.69	0	0	46.95	18.43	1.98	6.06	1.95
			433	0.37	0.84	57.02	4.62	0	0	38.42	13.89	2.58	6.01	1.94
1.5Au NH_3/*40*Si/Ti-MCM-36	15.3	1.1	453	(0.18)	(2.31)	(7.99)	(87.88)	(0)	(0)	(4.18)	(16.8)	(1.1)	(3.55)	(0.32)
				0.29	1.63	16.81	68.48	0	0	14.29	13.35	2.32	5.65	0.3
1.5Au NH_3/*100*Si Ti-MCM-36	30	0.74	453	(0.43)	(2.32)	(18.7)	(79.31)	(0)	(0)	(1.87)	(10.34)	(4.2)	(7.59)	(1.15)
				0.36	2.13	16.82	80.86	0	0	2.34	10.67	3.41	6.36	0.96
1.5Au NH_3/*160*Ti-MCM-36	94	0.38	453	(0.04)	(0.49)	(8.5)	(73.47)	(0)	(0)	(17.69)	(3.45)	(1.21)	(0.8)	(0.21)
				0.19	0.59	31.39	56.48	0	0	12.18	3.97	5.26	3.64	0.96

Reaction condition: 0.25 g catalysts, 433~498 K, space velocity: 7000 mL min^{-1} g_{cat}^{-1} [b] PO: propylene oxide, PA: propanal, ACR: acrolein, ACE: acetone.

The catalystic performance data in the bracket is collect after 10 min reaction; the other data is from the average of 6 h reaction.

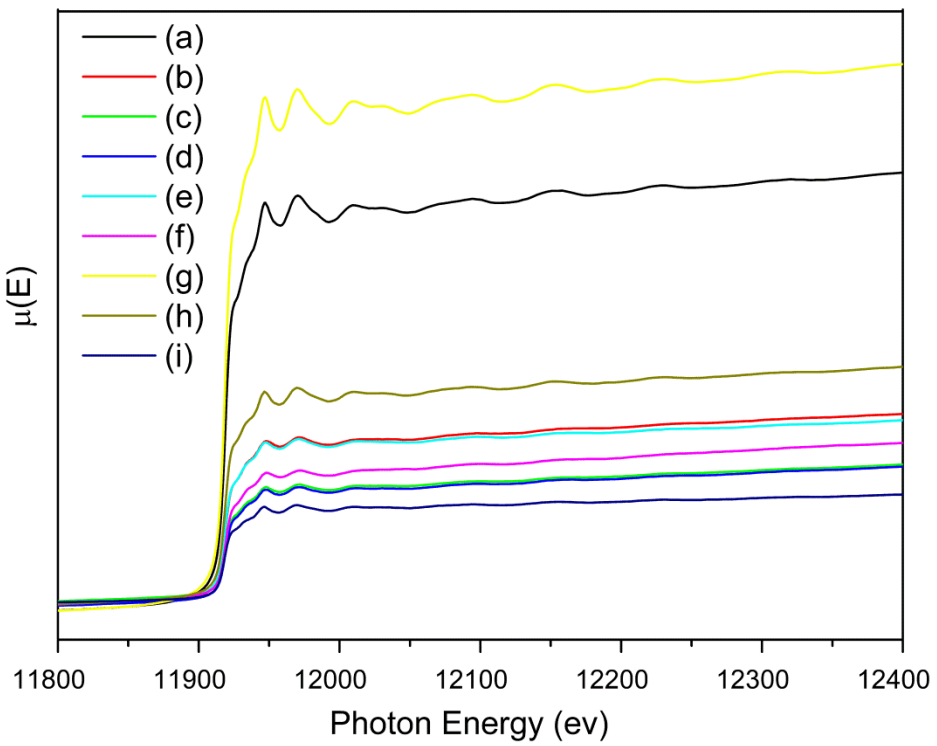

Figure S1. Au L_{III}-edge XAFS spectra collected in the fluorescence mode of the samples (a) 4.5Au/*100*Si/Ti-MCM-36, (b) 3Au/*100*Si/Ti-MCM-36, (d) 1.5Au/*100*Si/Ti-MCM-36, (d) 1Au/*100*Si/Ti-MCM-36, (e) 1.5Au/*160*Si/Ti-MCM-36, (f) 1.5Au/*40*Si/Ti-MCM-36, (g) 1.5AuNH_3/*40*Si/Ti-MCM-36, (h) 1.5AuNH_3/*100*Si/Ti-MCM-36, (i) 1.5AuNH_3/*160*Si/Ti-MCM-36.

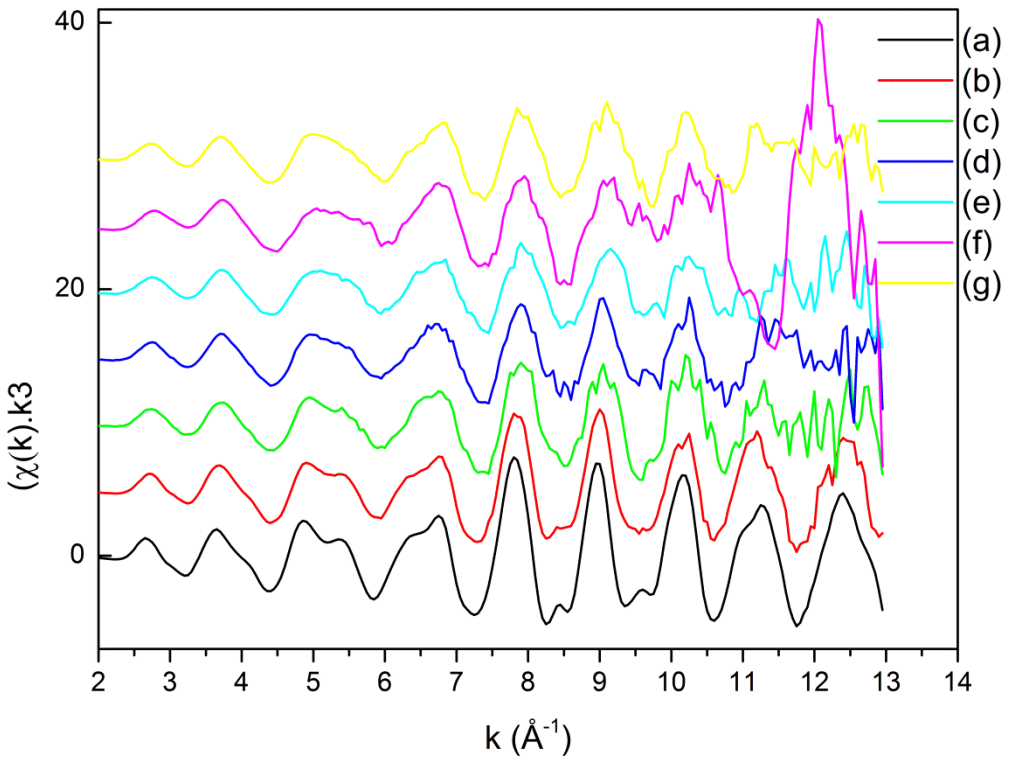

Figure S2(A). Au L_{III}-edge k3 weighted EXAFS spectra of (a) gold foil, and the samples prepared using NaOH as neutralization regent: (b) 4.5Au/*100*Si/Ti-MCM-36, (c) 3Au/*100*Si/Ti-MCM-36, (d) 1.5Au/*100*Si/Ti-MCM-36, (e) 1Au/*100*Si/Ti-MCM-36, (f) 1.5Au/*160*Si/Ti-MCM-36 and (g) 1.5Au/*40*Si/Ti-MCM-36.

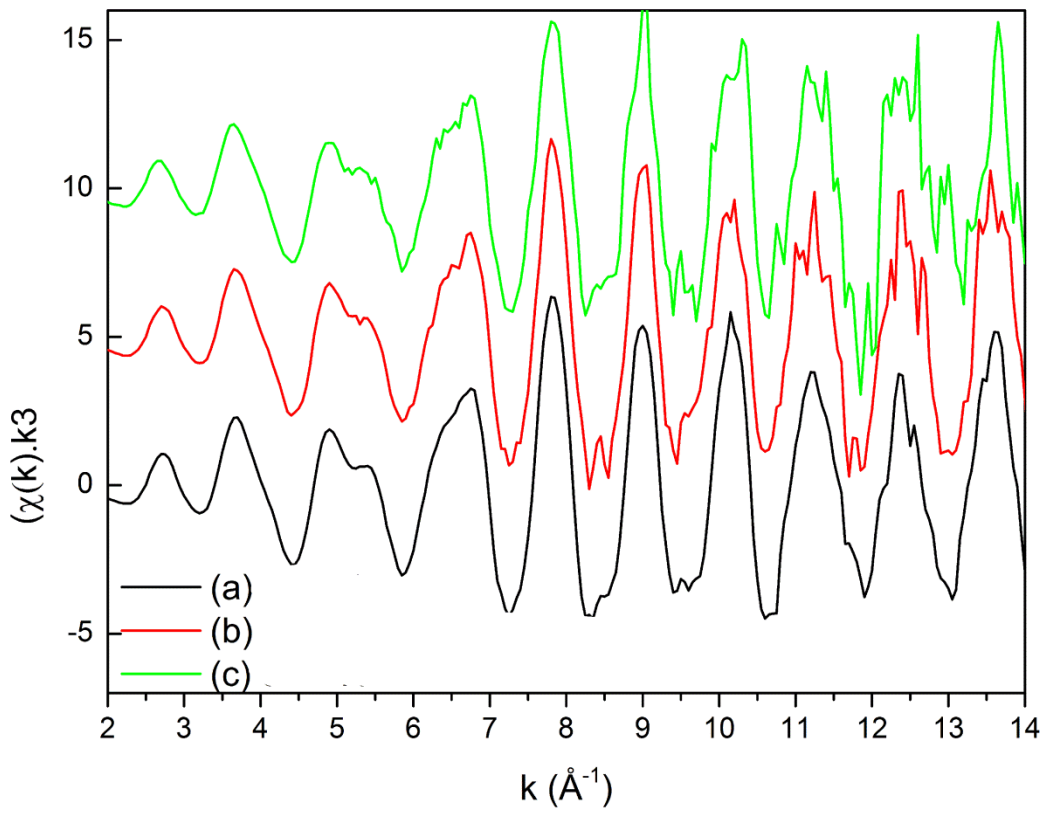

Figure S2(B). Au L_{III}-edge k3 weighted EXAFS spectra of (a) 1.5AuNH$_3$/*40*Si/Ti-MCM-36, and the samples prepared using NH_3 as neutralization regent: (b) 1.5AuNH$_3$/*100*Si/Ti-MCM-36 and (c) 1.5AuNH$_3$/*160*Si/Ti-MCM-36.

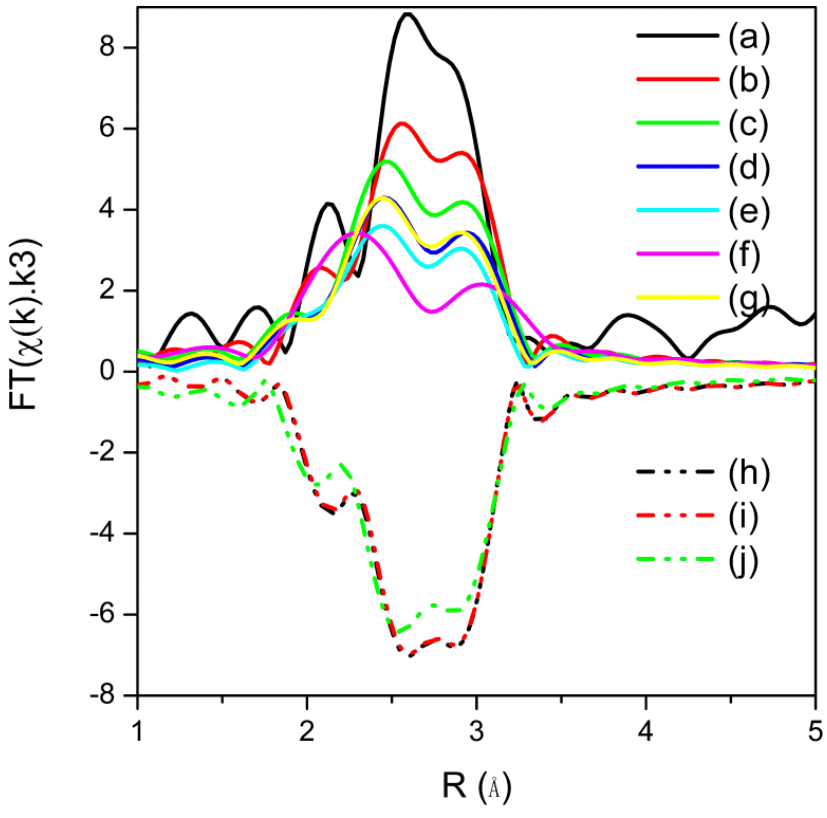

Figure S3. EXAFS of the Au L_{III}-edge curve fitting results of magnitude component of the χ(k)*k3 weighted in R space after applying a window around the first shell from 1.6~3.6 Å. (a) gold foil, (b) 4.5Au/*100*Si/Ti-MCM-36, (c) 3Au/*100*Si/Ti-MCM-36, (d) 1.5Au/*100*Si/Ti-MCM-36, (e) 1Au/*100*Si/Ti-MCM-36, (f) 1.5Au/*160*Si/Ti-MCM-36, (g) 1.5Au/*40*Si/Ti-MCM-36, (h) 1.5$AuNH_3$/*40*Si/Ti-MCM-36(vertical value multiple -1), (i) 1.5$AuNH_3$/*100*Si/Ti-MCM-36(vertical value multiple -1), (j) 1.5$AuNH_3$/*160*Si/Ti-MCM-36(vertical value multiple -1).

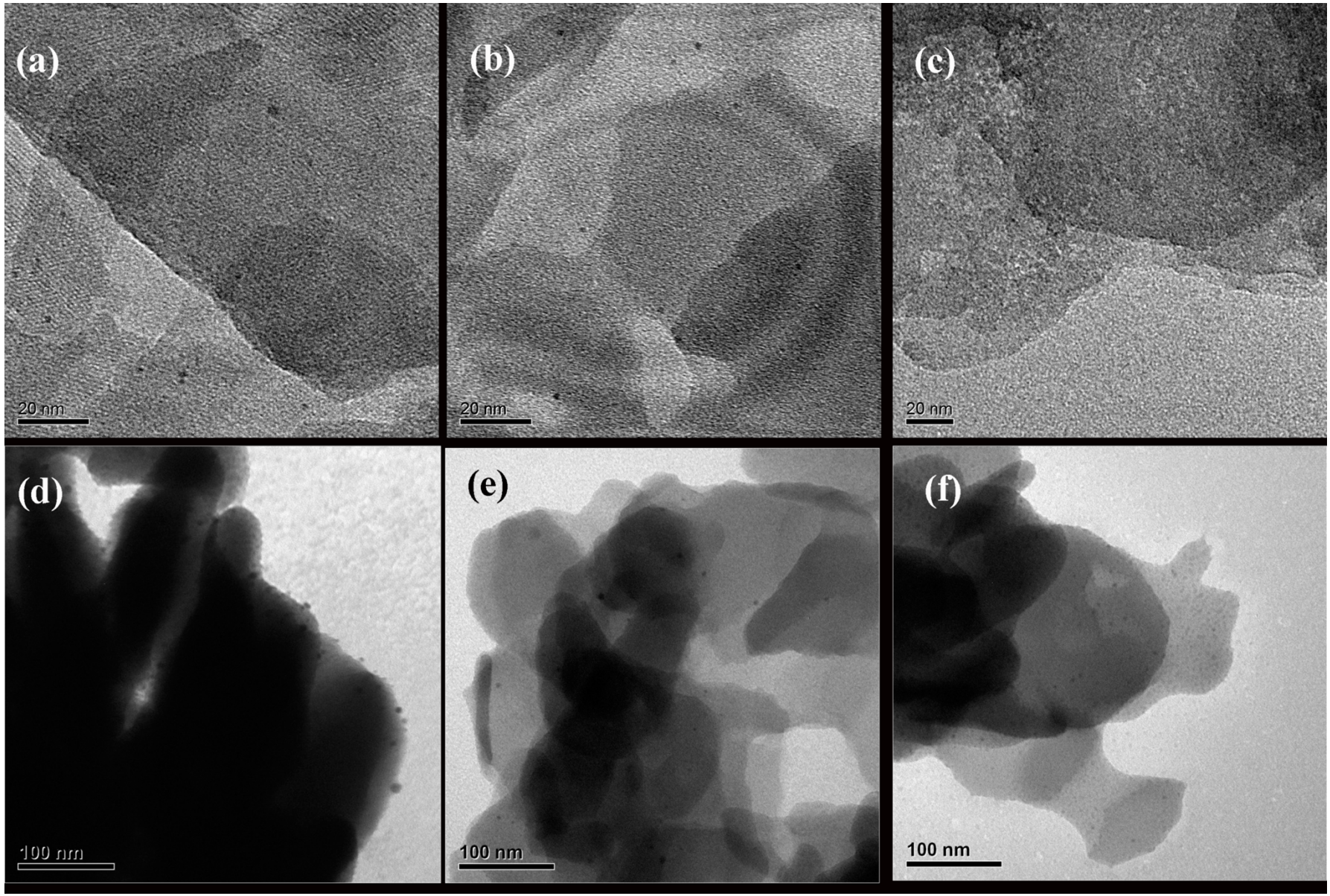
(a)
20 nm
(b)
20 nm
(c)
20 nm
(d)
100 nm
(e)
100 nm
(f)
100 nm

Figure. S4. TEM images of gold nanoparticles of (a) 1.5Au/*40*Si/Ti-MCM-36, (b) 1.5Au/*100*Si/Ti-MCM-36, (c) 1.5Au/*160*Si/Ti-MCM-36, (d) 1.5AuNH_3/*40*Si/Ti-MCM-36, (e) 1.5AuNH_3/*100*Si/Ti-MCM-36, (f) 1.5AuNH_3/*160*Si/Ti-MCM-36