Electronic Supplementary Information

Ag supported on alumina for the epoxidation of 1-hexene with molecular oxygen: the effect of Ag^{+}/Ag^{0}

Jingzhao Ren, [ac] Liancheng Wang,*[a] Penghui Li, [ac] Xiangying Xing, [ac] Huixiang Wang, [a] and Baoliang Lv *[ab]

[a] State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan 030001, China.

E-mail: wanglc@sxicc.ac.cn, lbl604@sxicc.ac.cn

[b] State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering, Ningxia University, Yinchuan 750021, China.

[c] University of Chinese Academy of Sciences, Beijing 100049, China

Experimental

The calculation equations on the yield of the products (X_i) and 1-hexene conversion were followed the Huang et al.[1], as follows:

$$X_i = \frac{N_i * n_{compounds}/6}{n_{1\text{-Hexene}}} \times 100\% \quad (1)$$

$$Conversion = \frac{\sum n * C_{n\ Compounds}/6}{n_{1\text{-Hexene}}} \times 100\% \quad (2)$$

Where N_i represents the number of carbon atoms for different compounds, $n_{compounds}$ represents the molar mass for different compounds, $n_{1\text{-hexenen}}$ represents initial of 1-hexene.

Results and discussion

Table S1 Ag content of the Ag/PBAs catalysts

Sample	Ag content (wt. %)*
Ag/PBAs 250	1.00
Ag/PBAs 300	0.96
Ag/PBAs 350	1.32
Ag/PBAs 400	0.90
Ag/PBAs 450	1.12

* Determined by ICP-AES measurement

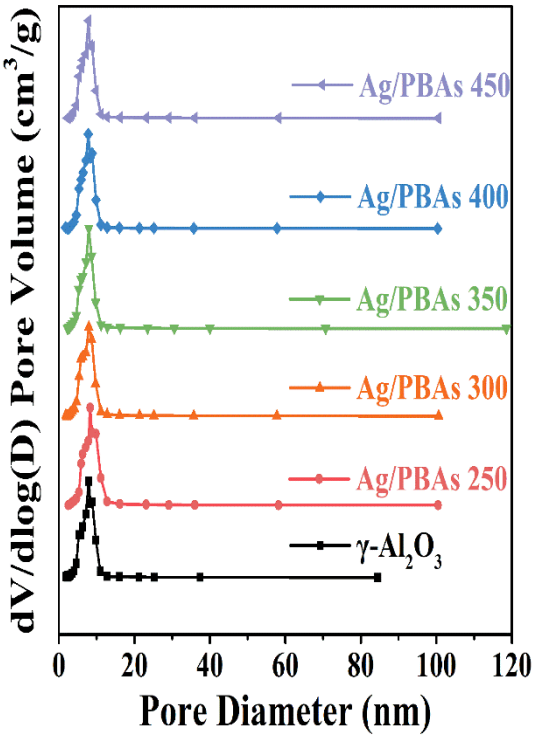

Fig. S1 Pore size distribution plots of pure PBAs and Ag/PBAs catalysts

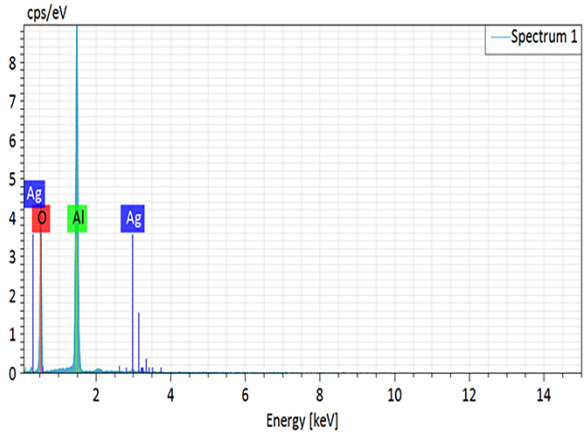

Fig. S2 Spectrum of elementary of Ag/PBAs 350.

Table S2 Elementary analysis results of Ag/PBAs 350.

Element	Weight (%)	Atomic (%)
O	34.1	62.4
Al	34.2	37.2
Ag	1.4	0.4

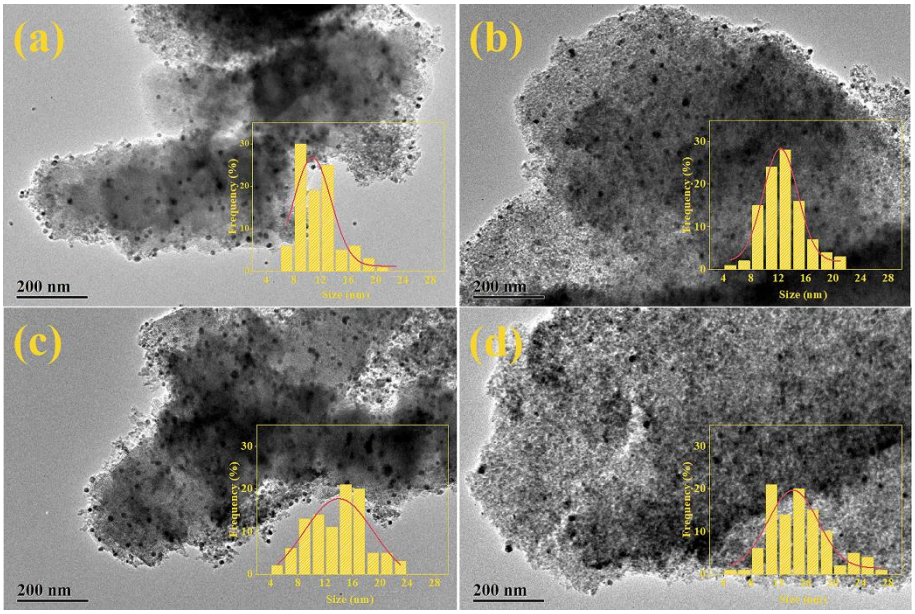

Fig. S3 TEM images of (a) Ag/PBAs 250, (b) Ag/PBAs 300, (c) Ag/PBAs 400, (d) Ag/PBAs 450

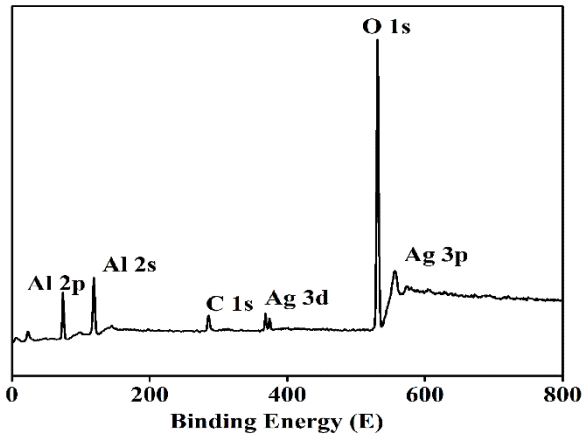

Fig. S4 XPS survey of Ag/PBAs 350

Table S3 Experimental results of different TBHP additions

TBHP amount (mmol)	0	0.2	0.4	0.8
Conversion (%)	0.43	8.18	13.84	14.03
Product yield (%)				
1,2-Epoxyhexane	0.03	3.29	6.08	4.71
1-Hexen-3-one	0.04	0.30	0.79	0.64
1-Hexen-3-ol	0.03	0.80	0.90	0.42
2-Hexenal	0.03	0.22	0.34	0.46
2-Hexenoic acid	0.12	0.22	0.33	0.87
1,2-Hexanediol	0.01	0.31	0.62	0.49
1-Hydroxyhexan-2-one	0.03	0.43	0.50	2.15
Valeraldehyde	0.01	0.23	0.32	0.45
Valeric acid	0.10	0.54	0.82	0.88
CO	0.01	0.11	0.09	0.13
CH_4	< 0.01	0.01	0.01	0.11
CO_2	< 0.01	0.24	0.34	0.28
Others [b]	0.02	1.49	2.71	2.43

[a] Reaction conditions: 1-hexene (4 mmol), 80 mg catalysts, 6 h, 140 °C, 0.3 MPa O_2

[b] Others include at least 15 unidentified products with yields less than 0.3%

Table S4 Experimental results of different reaction temperatures

Reaction temperature (℃) [a]	80	100	120	140
Conversion (%)	2.72	4.14	11.68	13.84
Product yield (%)				
1,2-Epoxyhexane	0.22	0.95	4.29	6.08
1-Hexen-3-one	0.43	0.52	1.16	0.79
1-Hexen-3-ol	0.99	1.05	1.49	0.90
2-Hexenal	0.30	0.22	0.46	0.34
2-Hexenoic acid	0.17	0.24	0.94	0.33
1,2-Hexanediol	0.02	0.12	0.57	0.62
1-Hydroxyhexan-2-one	0.01	0.06	0.37	0.50
Valeraldehyde	0.12	0.14	0.35	0.32
Valeric acid	0.05	0.12	0.49	0.82
CO	< 0.01	0.01	0.02	0.09
CH_4	< 0.01	< 0.01	< 0.01	0.01
CO_2	0.01	0.09	0.07	0.34
Others	0.39	0.65	1.48	2.71

[a] Reaction conditions: 1-hexene (4 mmol), TBHP (0.4 mmol), 80 mg catalysts, 6 h, 0.3 MPa O_2

Table S5 Experimental results of different oxygen partial pressures

Oxygen partial pressures (MPa) [a]	0.1	0.3	0.5
Conversion (%)	5.23	13.84	12.62
Product yield (%)			
1,2-Epoxyhexane	1.70	6.08	4.18
1-Hexen-3-one	0.19	0.79	0.35
1-Hexen-3-ol	1.14	0.90	0.44
2-Hexenal	0.23	0.34	0.76
2-Hexenoic acid	0.18	0.33	0.35
1,2-Hexanediol	0.21	0.62	0.50
1-Hydroxyhexan-2-one	0.25	0.50	0.96
Valeraldehyde	0.30	0.32	0.17
Valeric acid	0.25	0.82	0.66
CO	< 0.01	0.09	0.29
CH_4	< 0.01	0.01	0.04
CO_2	0.01	0.34	0.80
Others	0.75	2.71	3.13

[a] Reaction conditions: 1-hexene (4 mmol), TBHP (0.4 mmol), 80 mg catalysts, 6 h, 140 °C

Table S6 Experimental results of Ag/PBAs catalysts calcined at different temperatures.

Catalyst [a]	Ag/PBAs 250	Ag/PBAs 300	Ag/PBAs 350	Ag/PBAs 400	Ag/PBAs 450
Conversion (%)	7.22	7.80	13.84	10.38	10.69
Product yield (%)					
1,2-Epoxyhexane	2.15	3.15	6.08	4.05	3.44
1-Hexen-3-one	0.21	0.27	0.79	0.33	0.34
1-Hexen-3-ol	0.94	0.61	0.90	0.83	0.73
2-Hexenal	0.16	0.19	0.34	0.21	0.19
2-Hexenoic acid	0.36	0.20	0.33	0.29	0.34
1,2-Hexanediol	0.42	0.45	0.62	0.55	0.65
1-Hydroxyhexan-2-one	0.41	0.53	0.50	0.46	0.77
Valeraldehyde	0.28	0.24	0.32	0.36	0.35
Valeric acid	0.45	0.71	0.82	0.89	0.84
CO	0.10	0.10	0.09	0.13	0.14
CH_4	0.02	0.02	0.01	0.04	0.02
CO_2	0.24	0.17	0.34	0.35	0.19
Others	1.46	1.72	2.71	1.90	2.68

[a] Reaction conditions: 1-hexene (4 mmol), TBHP (0.4 mmol), 80 mg catalysts, 6 h, 140 °C, 0.3 MPa O_2

Reference

1 W. Xiong, X. Gu, Z. Zhang, P. Chai, Y. Zang, Z. Yu, D. Li, H. Zhang, Z. Liu and W. Huang, Nat. Commun., 2021, 12, 5921.