

Supplementary Information

Selective hydrodeoxygenation of lignin oil to valuable phenolics over Au/Nb₂O₅ in water

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I. Figures

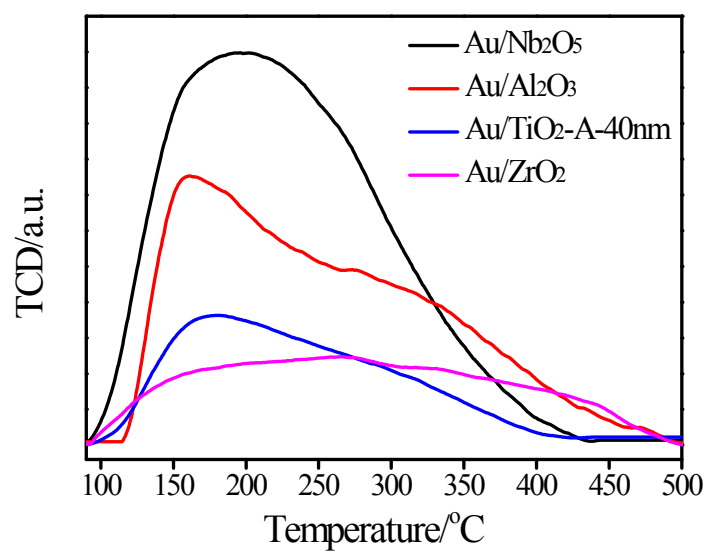


Fig. S1 NH₃-TPD profiles of Au/Nb₂O₅, Au/Al₂O₃, Au/TiO₂-A-40nm and Au/ZrO₂.

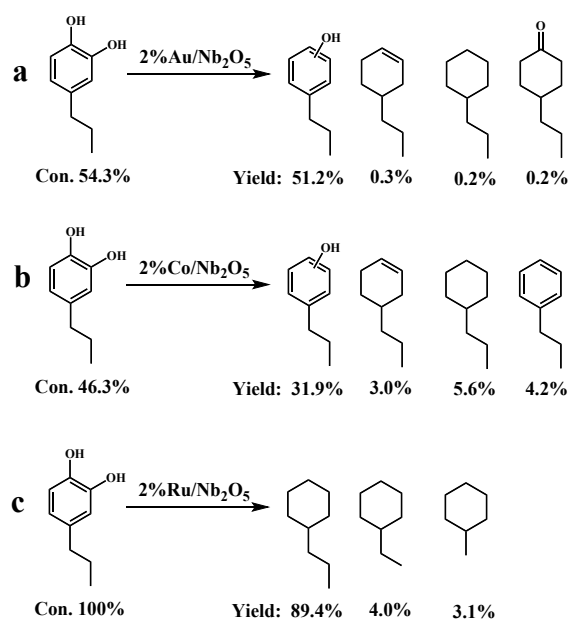


Fig. S2 Reaction results for the hydrodeoxygenation of 4-propylcatechol over different Au-based catalysts in a batch reactor. Reaction condition: 4-propylcatechol (0.5 g), catalyst (0.2 g), deionized water (10 mL), 300 °C, 2 h and initial H₂ pressure of 6.5 MPa.

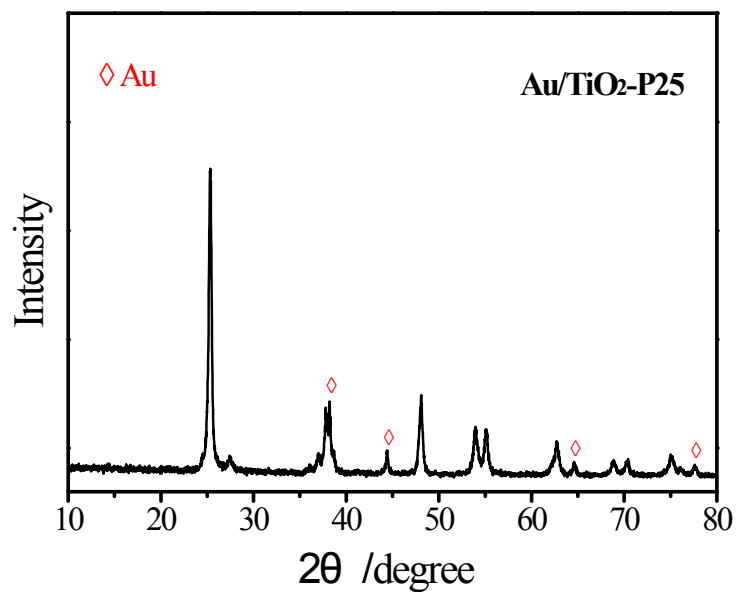


Fig. S3. XRD patterns of Au/TiO₂-P25.

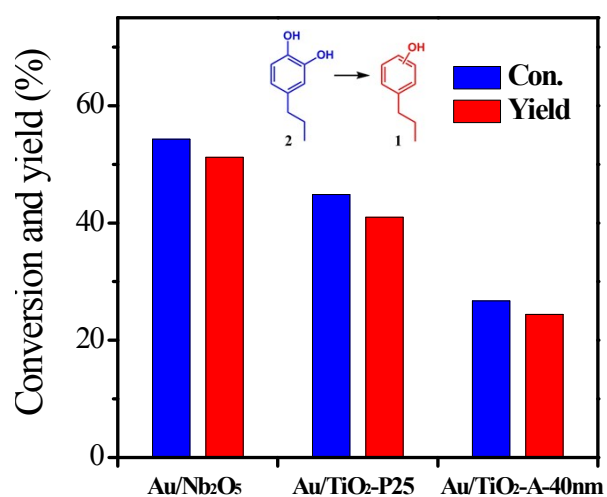
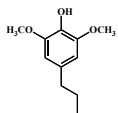
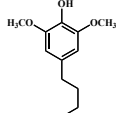
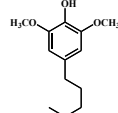
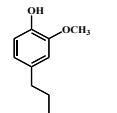
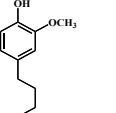
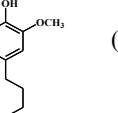


Fig. S4 Reaction results for the hydrodeoxygenation of 4-propylcatechol over different Au-based catalysts in a batch reactor. Reaction condition: 2-methoxy-4-propylphenol (0.5 g), catalyst (0.2 g), deionized water (10 mL), 300 °C, 2h and initial H₂ pressure of 6.5MPa.

II. Tables

Table S1. The component of various lignin oils.

Entry	Lignin oil	Component (wt %)						Total (wt %)
								
1	beech	54.5	0.7	0.5	18.3	0.4	0.4	74.8
2	birch	45.6	2.0	0.7	17.6	1.2	0.4	67.4
3	pine	35.4	1.6	0.5	35.6	1.2	0.6	74.9
4	cornstalk	23.1	3.7	0.7	21.9	1.7	0.8	52.0

The other components of lignin oil are polyhydric alcohols.

Table S2. Summary of physicochemical properties and ICP analysis results of Au/TiO₂-P25.

Catalyst	Surface area (m ² g ⁻¹)	Pore volume (cm ³ g ⁻¹)	Pore size (nm)	Au loading ^a (wt%)
Au/TiO ₂ -P25	21	0.207	17.4	2.0

^a Determined by ICP-AES.

Table S3. Results of full conversion of various types of lignocellulose

Lignocellulose		beech	birch	pine	cornstalk
Lignin oil (mg) ^a		98	152	100	84
Monomer yield (%) ^b		76	67	75	52
Monomer distribution ^c	1S	25	26	48	50
	2S	0	2	2	3
	3S	0	1	0	2

1G	73	68	47	37
2G	1	3	2	7
3G	1	1	1	1

Reaction conditions: lignocellulose (1.0 g), 5%Ru/C (0.1 g), methanol (20 mL), 250°C, 3h, and initial H₂ pressure of 3MPa.

^aCalculated based on weighed of electronic scales.

^bMonomeryield=weightmonomers/weightlignin oil×100%

^c“1S”, “2S”, “3S”, “1G”, “2G” and “3G” sign 2-methoxy-4-propylphenol, 4-(3-hydroxypropyl)-2-methoxyphenol, 2-methoxy-4-(3-methoxypropyl)phenol, 2,6-dimethoxy-4-propylphenol, 4-(3-hydroxypropyl)-2,6-dimethoxyphenol and 2,6-dimethoxy-4-(3-methoxypropyl)phenol, respectively.

III. Experimental procedures.

The preparation process of lignin oil

Lignin oil was derived from raw lignocellulosic biomass by reductive depolymerization. In a typical experiment, 1.0 g of raw lignocellulosic biomass sawdust (beech, birch, pine or cornstalk), 0.1 g Ru/C and 20 mL methanol were loaded into a 50 mL Teflon-lined stainless-steel autoclave. The reactor was sealed, purged with H₂ three times and pressurized with 3 MPa at room temperature. The mixture was stirred at 800 rpm and the temperature was increased to 250 °C for 3h. After reaction, the autoclave was cooled in ice-water bath immediately. The lignin oil was obtained from reaction mixture by vacuum distillation to remove solvent.