

Supplementary Materials: Selective Alkylation of Benzene with Propane over Bifunctional Pd-Acid Catalysts

Abdullah Alotaibi, Sophie Hodgkiss, Elena F. Kozhevnikova and Ivan V. Kozhevnikov

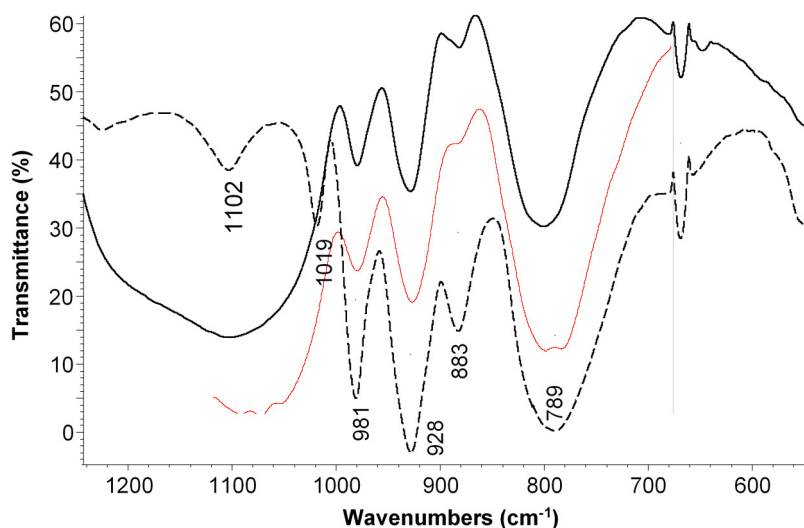


Figure S1. FTIR spectra of bulk HSiW (dashed line), fresh 2%Pd/25%HSiW/SiO₂ (solid black line), and spent 2%Pd/25%HSiW/SiO₂ (red line).

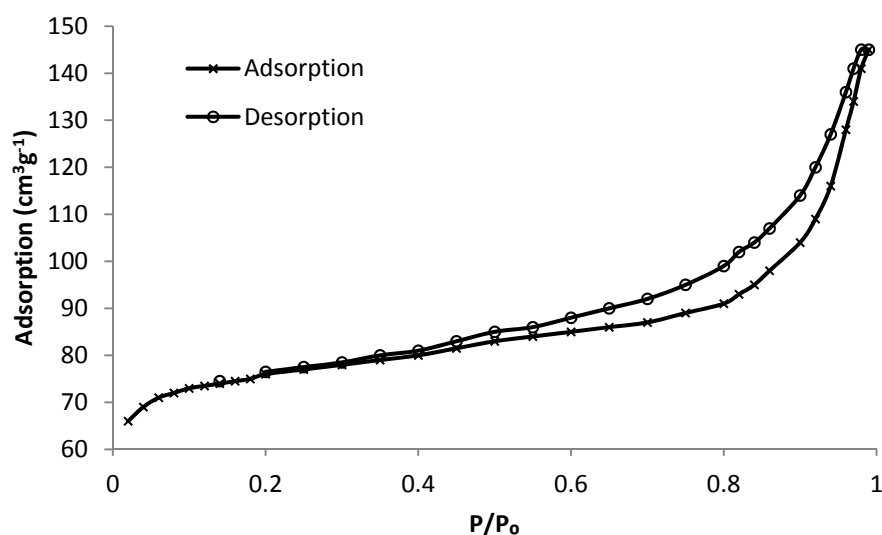


Figure S2. Nitrogen adsorption (x) and desorption (o) isotherms for 2%Pd/HZSM-5.

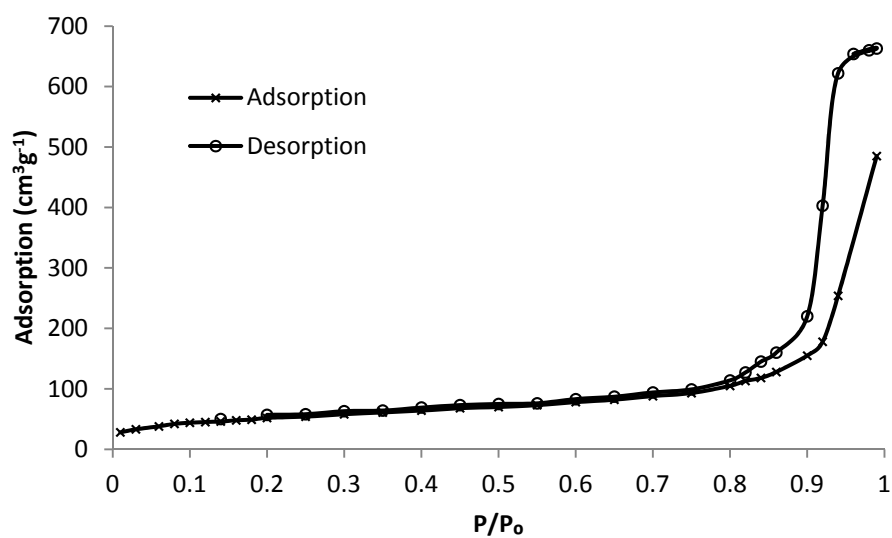


Figure S3. Nitrogen adsorption (×) and desorption (○) isotherms for 2%Pd/25%HSiW/SiO₂.

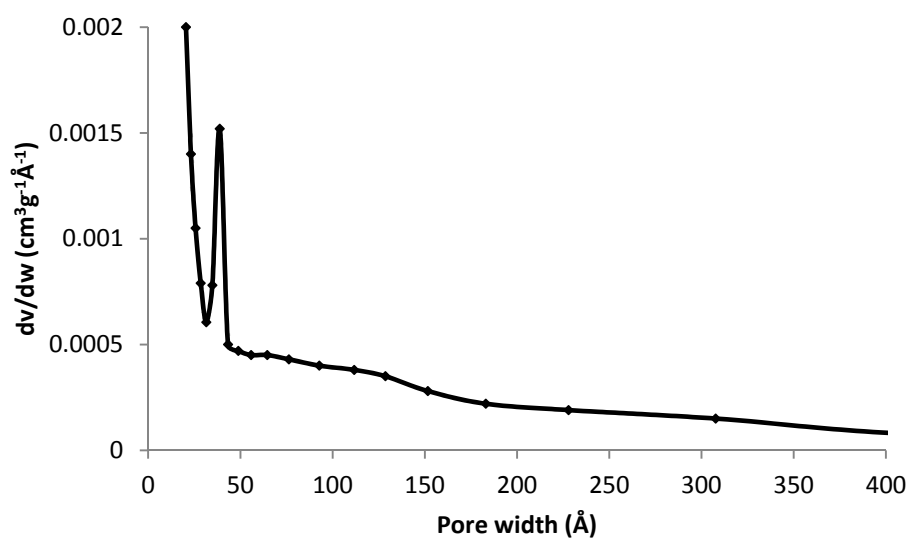


Figure S4. BJH desorption pore size distribution for 2%Pd/HZSM-5.

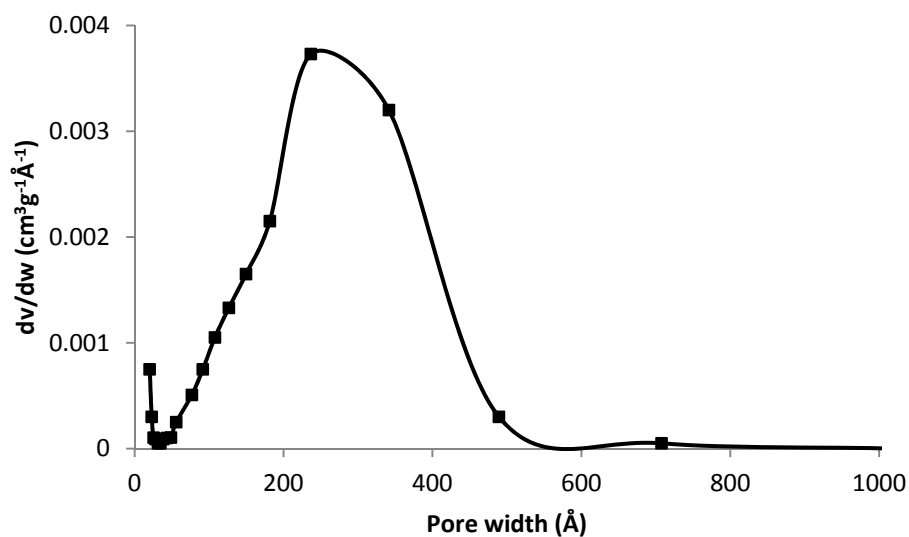


Figure S5. BJH desorption pore size distribution for 2%Pd/25%HSiW/SiO₂.

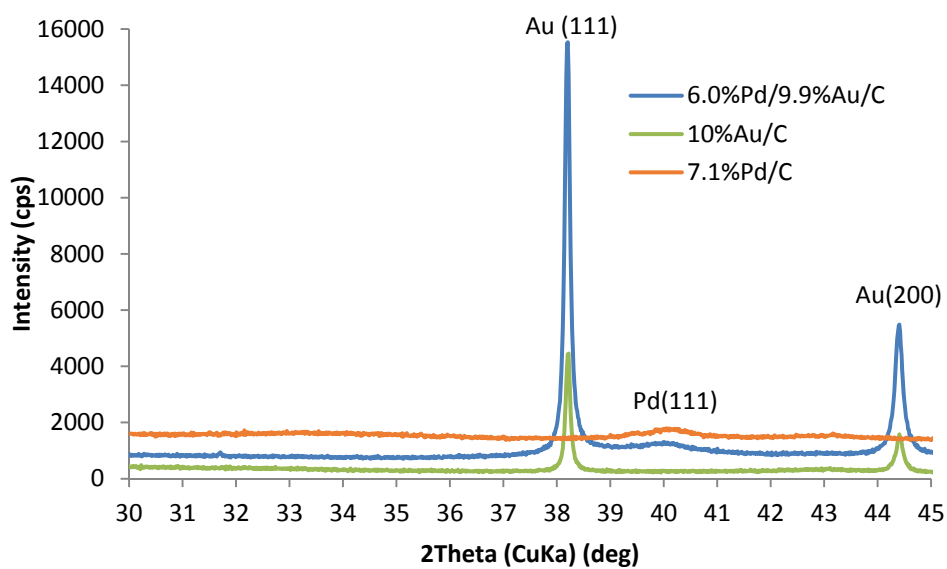


Figure S6. XRD of carbon-supported metal catalysts: 6.0%Pd/9.9%Au/C (blue), 10%Au/C (green), and 7.1%Pd (beige).

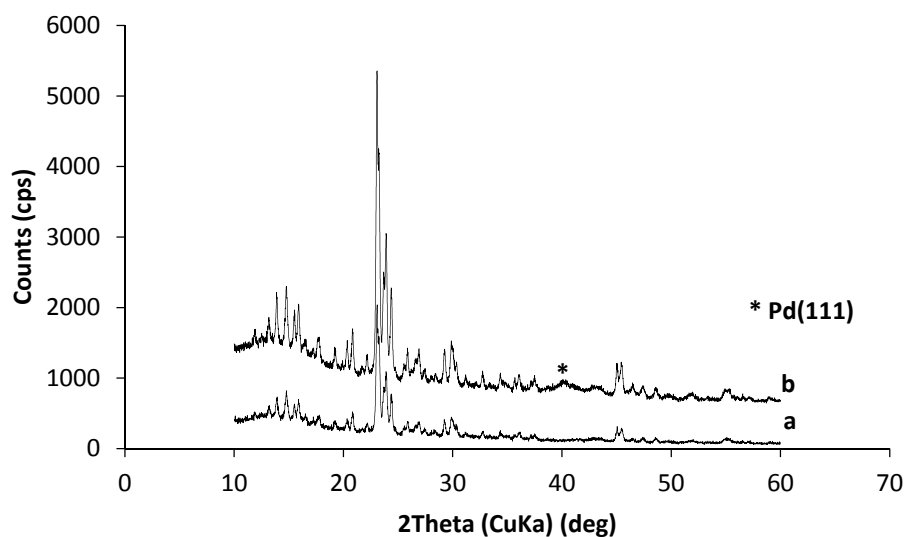


Figure S7. XRD patterns for zeolite catalysts: (a) HZSM-5 and (b) 2%Pd/HZSM-5 (Si/Al = 10).

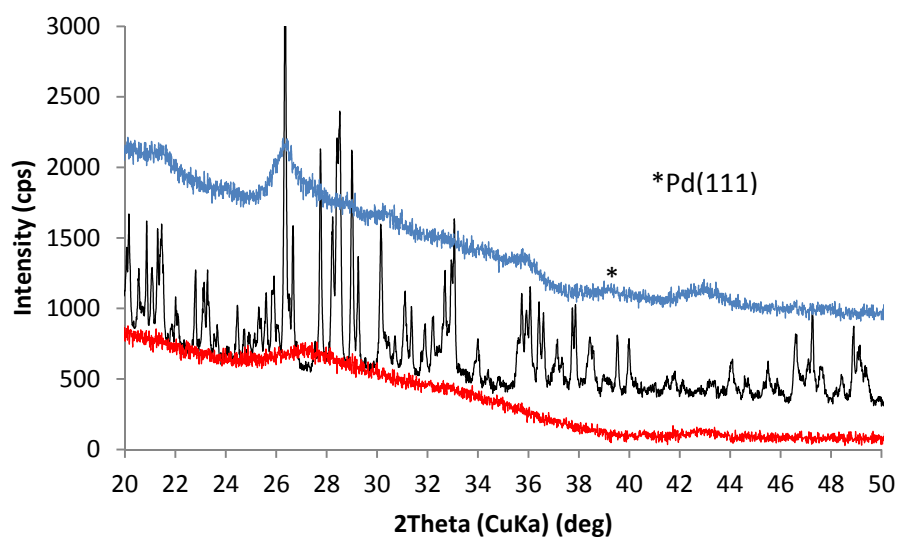


Figure S8. XRD patterns (CuK α radiation) for bulk HSiW (black line), 25%HSiW/SiO₂ (red line), and 2.0%Pd/25%HSiW/SiO₂ (blue line).

Table S1. Alkylation of benzene with propane over AuPd-HZSM-5 and AuPd-HSiW catalysts.^a

Catalyst	Conv. ^b (%)	Aromatic selectivity (%) ^c				
		MePh	EtPh	iPrPh	nPrPh	C ₉₊
1) 0.5%Au/HZSM-5	0.5	0	35.4	12.9	23.7	28.0
2) 5.0%Au/C+HZSM-5 (2.0%Au) ^d	0.4	0	30.0	18.3	36.5	15.2
3) PdAu/C+HZSM-5 (1.2%Pd, 2.0%Au) ^d	8.8	34.2	23.3	10.6	18.4	13.5
4) Pd/C+HZSM-5 (1.4%Pd) ^d	9.2	34.9	21.8	12.0	19.2	12.2
5) 10%Au/C+HSiW/SiO ₂ (2.0%Au) ^d	0.4	0	22.6	18.0	28.4	31.0
6) AuPd/C+HSiW/SiO ₂ (1.2%Pd, 2.0%Au) ^d	3.8	2.9	1.6	72.3	5.7	16.7
7) Pd/C+HSiW/SiO ₂ (1.4%Pd) ^d	3.7	0	2.0	74.2	6.7	17.1
8) AuPd/C+HSiW/SiO ₂ (1.2%Pd, 2.0%Au) ^e	5.8	6.5	2.7	70.9	14.3	5.6
9) Pd/C+HSiW/SiO ₂ (1.4%Pd) ^e	5.2	4.4	3.1	70.6	15.9	6.0

^a Reaction conditions: 300 °C, 1 bar pressure, 0.20 g catalyst, inlet molar ratio C₆H₆/C₃H₈ = 1:9, 10 mL min⁻¹ flow rate, W/F = 80 g h mol⁻¹; in situ catalyst pre-treatment at 300 °C/1 h in H₂ flow, 10 mL min⁻¹. ^b Benzene conversion at 3 h time on stream. ^c Selectivity to aromatic products including unidentified C₉₊ alkylbenzenes at 3 h time on stream. ^d Uniform physical mixture of 7.1%Pt/C or 9.9%Au/6.0%Pd/C with HZSM-5 or 25%HSiW/SiO₂. ^e Two catalyst beds: 7.1%Pd/C or 9.9%Au/6.0%Pd/C (0.04 g, top bed) and 25%HSiW/SiO₂ (0.16 g, bottom bed).