

Supplementary Information

Efficient cross-coupling of acetone with linear aliphatic alcohols over supported copper on a fluorite-type $\text{Pr}_2\text{Zr}_2\text{O}_7$

Suhyun Lim ^{1,†}, Minseok Kim ^{1,†}, Sang Hyeok Ko ¹, Jae-Hong Lee ¹, Joon Hyun Baik ², and Young-Woong Suh ^{1,3,*}

¹ Department of Chemical Engineering, Hanyang University, Seoul 04763, Korea

² Department of Chemical and Biological Engineering, Sookmyung Women's University, Seoul 04310, Korea

³ Research Institute of Industrial Science, Hanyang University, Seoul 04763, Republic of Korea

*Corresponding: ywsuh@hanyang.ac.kr

[†]These authors contributed equally to this work.

Table S1. Conversion of butanol measured under different reaction conditions, where the reactant was 20 g with the butanol/acetone mole ratio of 2 and the catalyst used was 1 g.

Catalyst	Nominal Cu loading [wt%]	Temp. [°C]	Time [h]	Water content [wt%]	Number of cycle	Butanol conversion [mol%]	Associated figure
Cu/ <i>m</i> -ZrO ₂	5	240	20	0	-	56.2	Fig. 4
Cu/PrO _{1.83}	5					91.0	Fig. 4
Cu/Pr ₂ Zr ₂ O ₇	5					82.6	Fig. 4
	1					60.2	Fig. 6
	3					72.2	Fig. 6
	5		3			40.7	Fig. 8
			6			54.4	Fig. 8
			12			74.0	Fig. 8
			24			82.4	Fig. 8
			20	3		76.9	Fig. 9
				5		73.1	Fig. 9
				7		66.2	Fig. 9
				10		58.4	Fig. 9
	200	20	0	1 st	50.9	Fig. 10a	
				2 nd	48.6	Fig. 10a	
				3 rd	50.0	Fig. 10a	
				2 nd	79.3	Fig. 10b	
				3 rd	56.4	Fig. 10b	
				4 th	73.4	Fig. 10b	

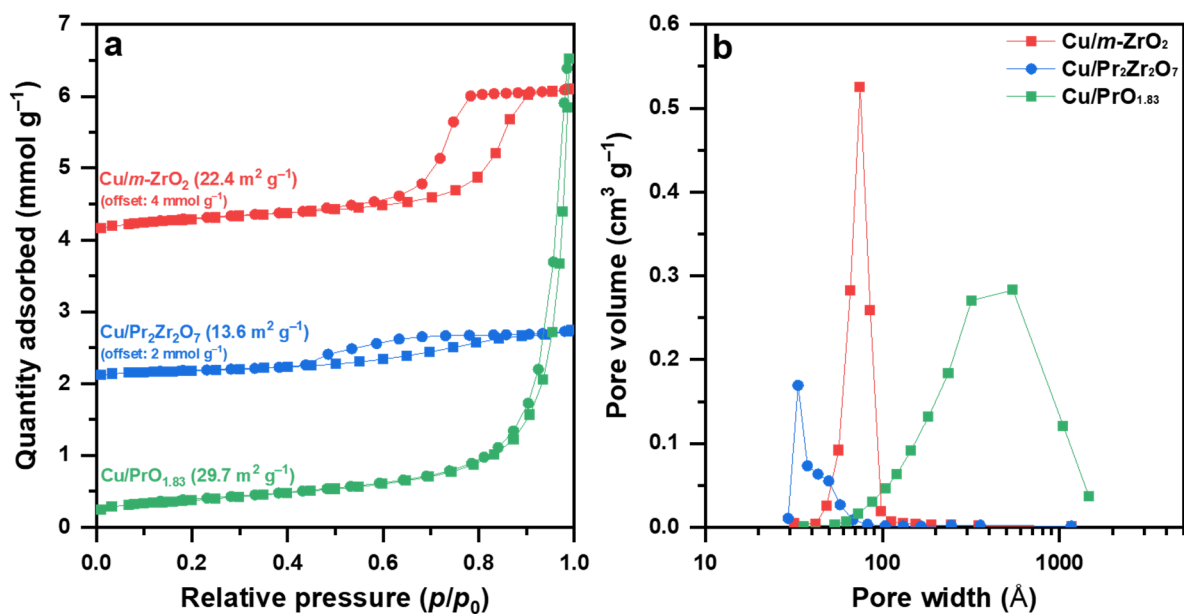


Figure S1. N₂ physisorption results of Cu/*m*-ZrO₂, Cu/PrO_{1.83}, and Cu/Pr₂Zr₂O₇ listed in Table 1: (a) BET isotherms and (b) pore size distribution curves.

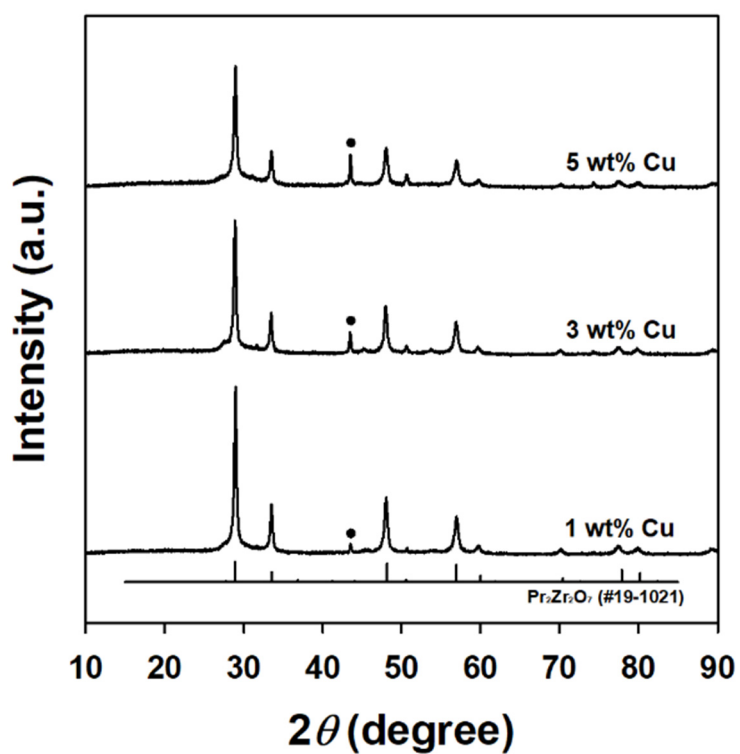
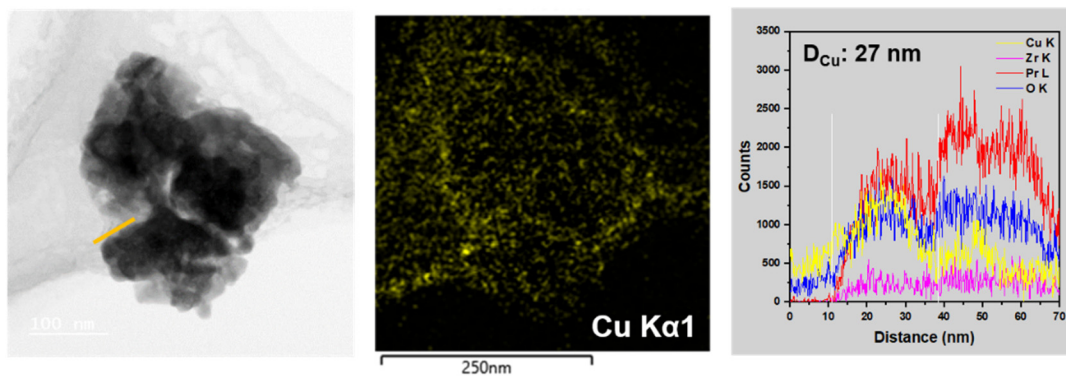
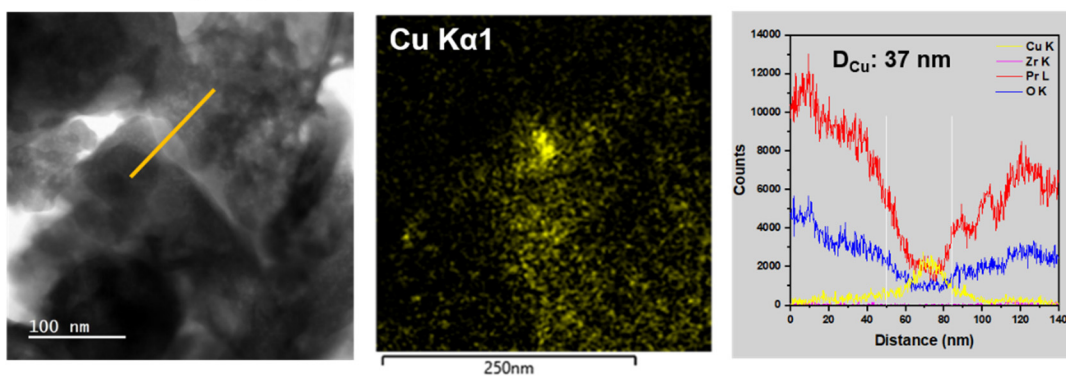


Figure S2. XRD patterns of the reduced Cu/Pr₂Zr₂O₇ of 1, 3, and 5 wt% Cu. The diffraction peak of Cu (111) is represented by the square symbol.

a 1Cu/Pr₂Zr₂O₇



b 3Cu/Pr₂Zr₂O₇



c 5Cu/Pr₂Zr₂O₇

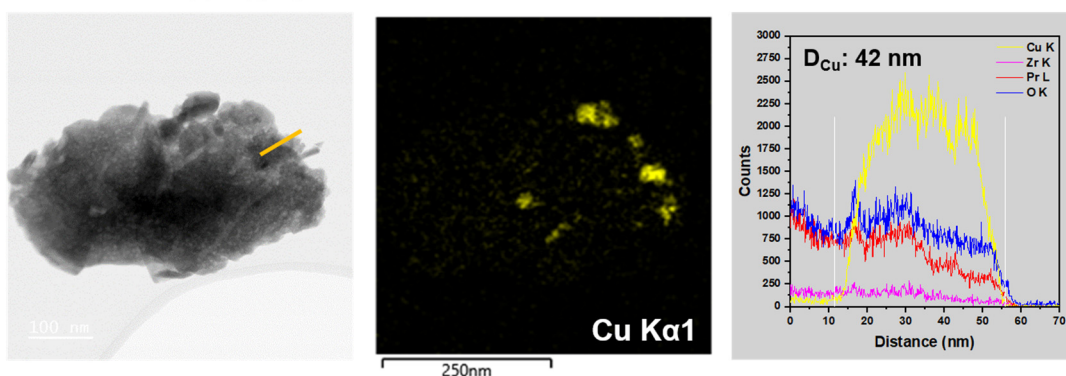


Figure S3. TEM images, Cu EDS mapping images, and line scanning results (obtained by tracking the orange line in the first image): (a) 1Cu/Pr₂Zr₂O₇, (b) 3Cu/Pr₂Zr₂O₇, and (c) 5Cu/Pr₂Zr₂O₇.