

The conversion of levulinic acid into γ -valerolactone using Cu-ZrO₂ catalysts

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Table S1. Theoretical Cu/Zr molar ratios and the measured ratios determined by ICP-AES

| Theoretical Cu/Zr Molar | Measured Cu/Zr |
|-------------------------|----------------|
| 0.25 | 0.27 |
| 0.50 | 0.50 |
| 0.75 | 0.80 |
| 1.00 | 0.99 |
| 1.25 | 1.25 |
| 1.50 | 1.53 |
| 2.00 | 2.04 |

Table S2. BET surface area for the catalysts prepared with different Cu/Zr ratios

| Theoretical Cu/Zr | BET surface area / m ² g ⁻¹ |
|-------------------|---|
| 0.25 | 23 |
| 0.50 | 18 |
| 0.75 | 32 |
| 1.00 | 149 |
| 1.25 | 90 |
| 1.50 | 86 |
| 2.00 | 81 |

Table S3. Particles sizes of catalysts prepared with different Cu/Zr ratio based on the most intense peak at 35° (hkl = (111)) using the Scherrer equation.

| Cu/Zr ratio | CuO particle size / nm |
|-------------|--|
| 0.25 | Unable to acceptably estimate particle size using the Scherrer equation |
| 0.50 | |
| 0.75 | |
| 1.00 | 11.0 |
| 1.25 | 8.3 |
| 1.50 | 20.0 |

Table S4. BET surface areas and particles sizes of catalysts prepared with different calcination temperatures. Particle sizes based on the most intense peak at 35° ($hkl = (111)$) using the Scherrer equation.

| Calcination temperature / $^\circ\text{C}$ | BET surface area / $\text{m}^2 \text{g}^{-1}$ | CuO particle size / nm |
|--|---|------------------------|
| 300 | 171 | 4.0 |
| 400 | 149 | 5.4 |
| 500 | 111 | 8.3 |
| 600 | 34 | 12.2 |
| 700 | 10 | 17.9 |
| 800 | 6 | 23.4 |

Table S5. BET surface areas and particles sizes of catalysts prepared with different precipitate ageing times. Particles sizes based on the most intense peak at 35° ($hkl = (111)$) using the Scherrer equation.

| Precipitates ageing time / h | BET surface area / $\text{m}^2 \text{g}^{-1}$ | CuO particle size / nm |
|------------------------------|---|---|
| 0 | 92.0 | 10.2 |
| 1 | 97.0 | 8.4 |
| 2 | 115 | 5.7 |
| 4 | 126 | 6.3 |
| 6 | 149 | 5.4 |
| 8 | 140 | 5.0 |
| 11 | 137 | Unable to acceptably estimate particle size using the Scherrer equation |
| 16 | 121 | |
| 24 | 116 | |

Table S6. Cu surface area determined by N_2O titration for Cu-ZrO₂ catalysts calcined at different temperatures.

| Calcination temperature / $^\circ\text{C}$ | Cu surface area / $\text{m}^2 \text{g}^{-1}$ |
|--|--|
| 300 | 1.7 |
| 400 | 4.1 |
| 500 | 0.7 |
| 600 | 4.1 |
| 700 | 1.0 |

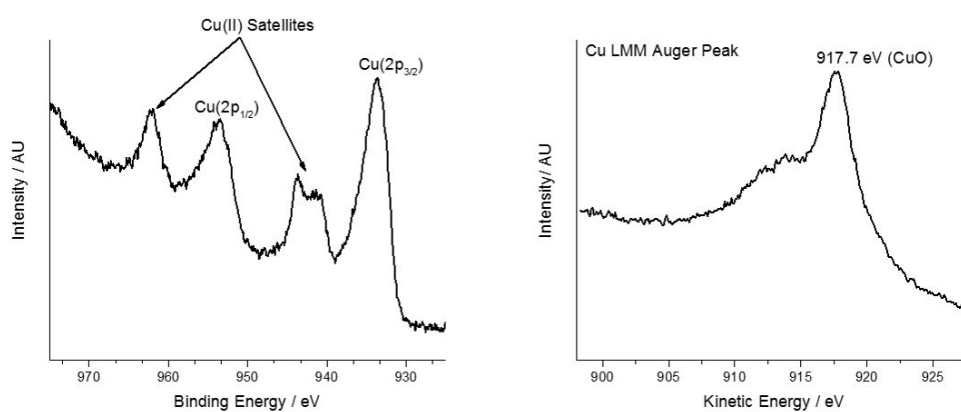


Figure S1. Typical XPS profile of CuO containing catalyst materials.

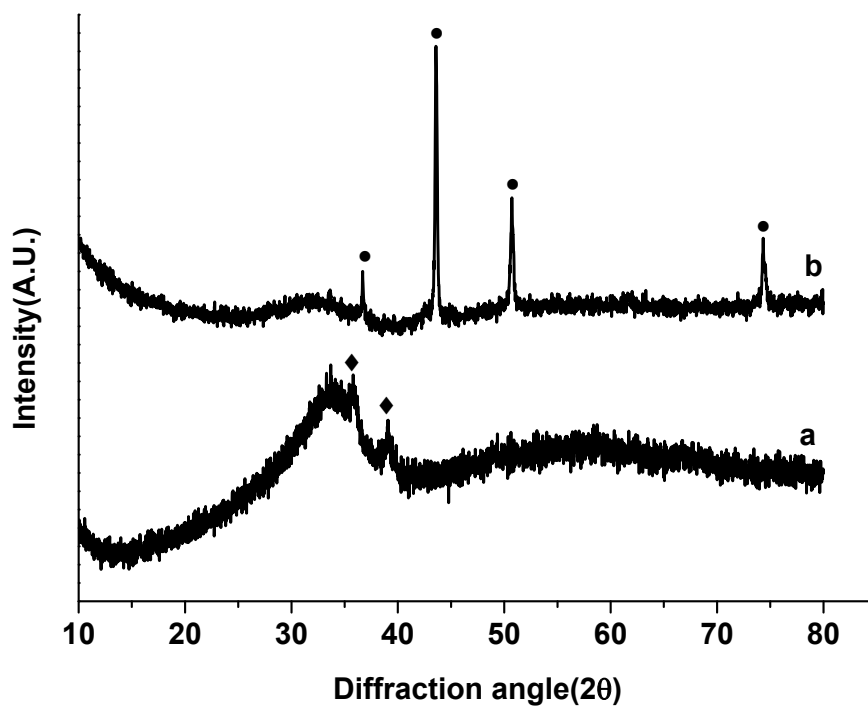


Figure S2. XRD patterns of the catalyst a) before and b) after reaction. \circ Cu, \bullet CuO

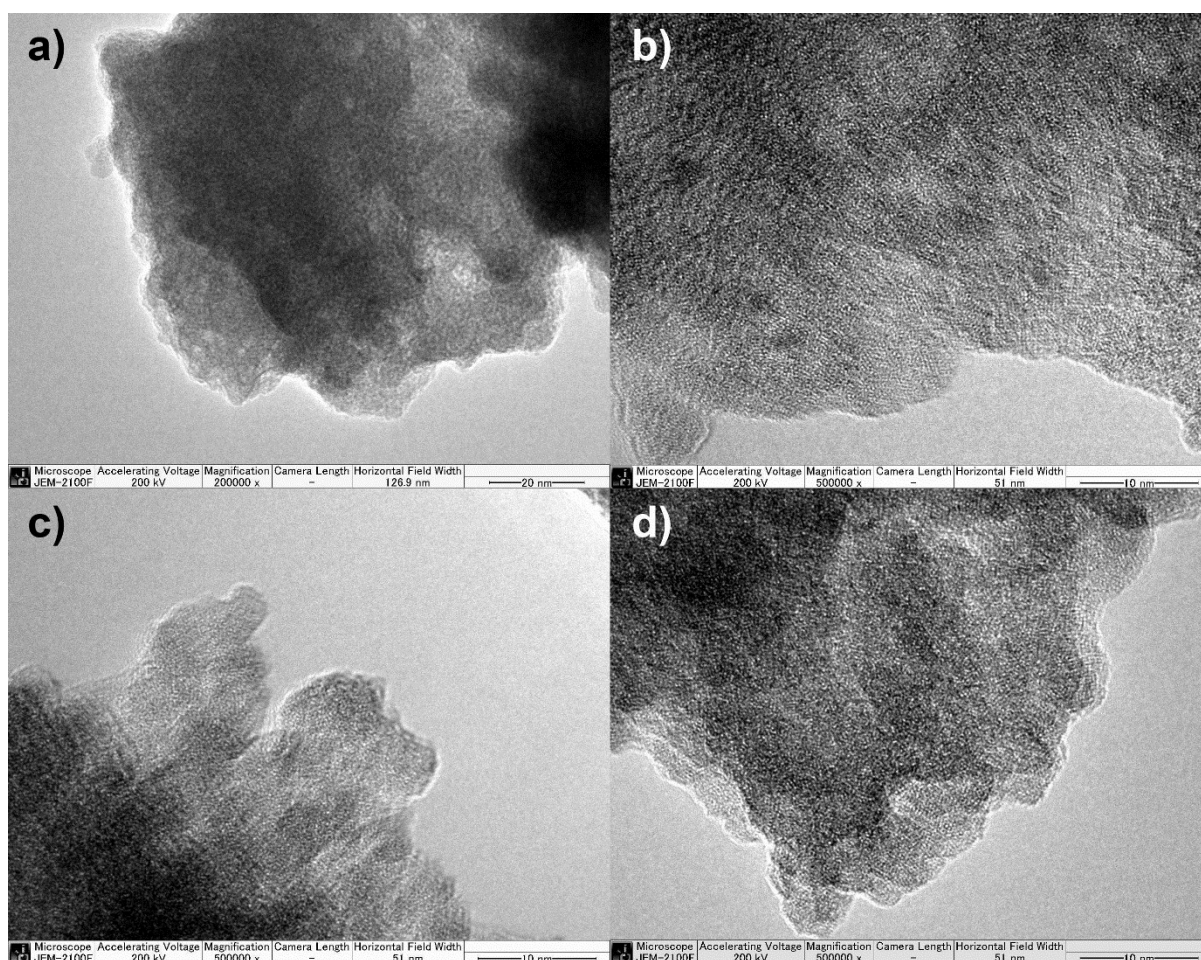


Figure S3: Tem images of Cu/ZrO₂ a) unaged, b) after calcination for 4h, c) 6h and d) 24h.