Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

Supplementary material for

Influence of La−doping on the CuO/ZrO_2 catalysts with different Cu content for hydrogenation of dimethyl oxalate to ethylene glycol

Jian Ding[a, b, c, *], Meihui Wang[a], Huimin Liu[a], Zhenfeng Wang[d], Xiaohui Guo[a], Gewen Yu[a, b, c], Yaxiong Wang[a, b, c]

[a] Inner Mongolia Key Laboratory of Coal Chemical Engineering & Comprehensive Utilization, School of Chemistry and Chemical Engineering, Inner Mongolia University of Science & Technology, Baotou 014010, Inner Mongolia, PR China

[b] Inner Mongolia Cooperative Innovation Center for Green Coal Mining & Green Utilization, Baotou 014010, Inner Mongolia, PR China

[c] Inner Mongolia Engineering Research Center of Coal Cleaning & Comprehensive Utilization, Baotou 014010, Inner Mongolia, PR China

[d] School of Materials and Metallurgy, Inner Mongolia University of Science & Technology, Baotou 014010, Inner Mongolia, PR China

[*] Corresponding author.
E-mail: dingjian@imust.edu.cn; Tel.: +86 0472 5953321.

Table S1. The input of raw materials needed for preparation of *w*CZ and *w*CLZ (g).

Catalyst	$Cu(NO_3)_2 \cdot 3H_2O$	$La(NO_3)_3 \cdot 6H_2O$	$Zr(NO_3)_4 \cdot 5H_2O$	SA
5CZ/**5CLZ**	0.1888/**0.1888**	-/**0.0312**	3.2668/**3.2259**	4.6409/**4.6172**
10CZ/**10CLZ**	0.3775/**0.3775**	-/**0.0312**	3.0490/**3.0081**	4.5733/**4.5489**
20CZ/**20CLZ**	0.7550/**0.7550**	-/**0.0312**	2.6134/**2.5726**	4.4379/**4.4141**
28CZ/**28CLZ**	1.0570/**1.0570**	-/**0.0312**	2.2650/**2.2241**	4.3296/**4.3057**
33CZ/**33CLZ**	1.2458/**1.2458**	-/**0.0312**	2.0472/**2.0063**	4.2619/**4.2382**
39CZ/**39CLZ**	1.4723/**1.4723**	-/**0.0312**	1.7858/**1.7450**	4.1807/**4.1573**
58CZ/**58CLZ**	2.1895/**2.1895**	-/**0.0312**	0.9583/**0.9174**	3.9235/**3.8986**

The exposed Cu surface area and Cu dispersion was measured by N_2O oxidation and followed H_2 reduction. Generally, catalysts (60 mg) were first reduced in 5% H_2/N_2 mixture at a flow rate of 30 mL min^{-1} with a ramping rate of 10 °C min^{-1} until 350 °C. The amount of hydrogen consumption in the first TPR (TPR1) was denoted as X. And then the reactor was purged with Ar to 50 °C. N_2O (30 mL min^{-1}) was injected to oxidize surface copper atoms to Cu_2O at 50 °C for 15 min. Subsequently, the reactor was flushed with Ar to remove the oxidant. Finally, another TPR experiment was performed in 5% H_2/N_2 at a flow rate of 30 mL min^{-1}. Hydrogen consumption in the second TPR (TPR1) was denoted as Y. The dispersion of Cu and exposed Cu surface area were calculated according to the equations which were shown below:

Reduction of all copper atoms:

$CuO + H_2 \rightarrow Cu + H_2O$, hydrogen consumption in the first TPR1 = X.

The decomposition of N_2O on the surface of metallic copper:

$2Cu + N_2O = N_2 + (Cu–O–Cu)s$.

Reduction of surface copper atoms only:

$Cu_2O + H_2 \rightarrow 2Cu + H_2O$, hydrogen consumption in this TPR2 = Y;

And the dispersion of Cu and exposed Cu surface area were calculated as [Eq. (1, 2)]:

$$\boldsymbol{D = \frac{2Y}{X} \times 100\%} \qquad (1)$$

$$\boldsymbol{S = \frac{2Y \times N_{av}}{X \times M_{Cu} \times 1.4 \times 10^{19}} = \frac{1353Y}{X}(m^2 - Cu/g - Cu)} \qquad (2)$$

where N_{av} is the Avogadro's constant, M_{Cu} is the relative atomic mass, 1.4×10^{19} comes from that an equal abundance of an average copper surface atom area of

0.0711 nm^2, equivalent to 1.4×10^{19} copper atoms m^{-2}.

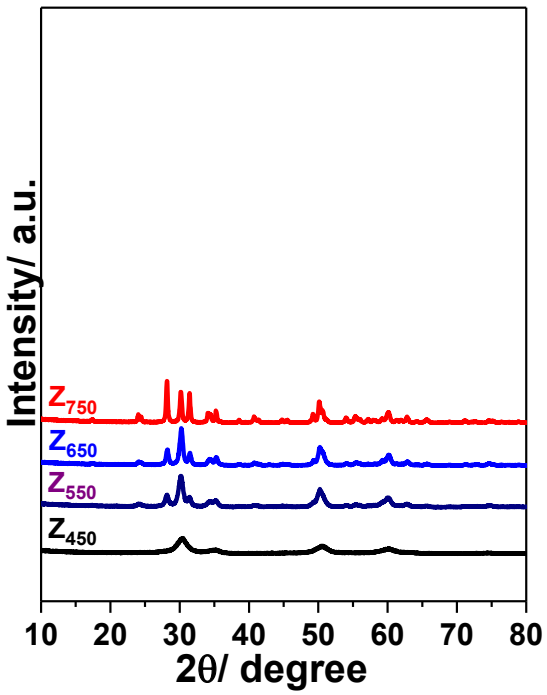

Figure S1. XRD patterns of the ZrO_2 powders calcined at 450, 550, 650, and 750 ^oC.

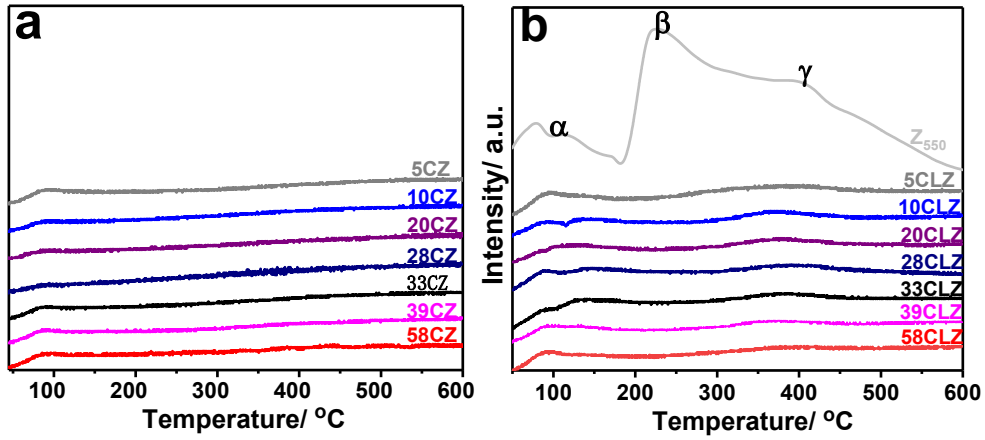

Figure S2. CO_2−TPD profiles of as-prepared catalysts (a: *w*CZ; b: *w*CLZ and standard ZrO_2).

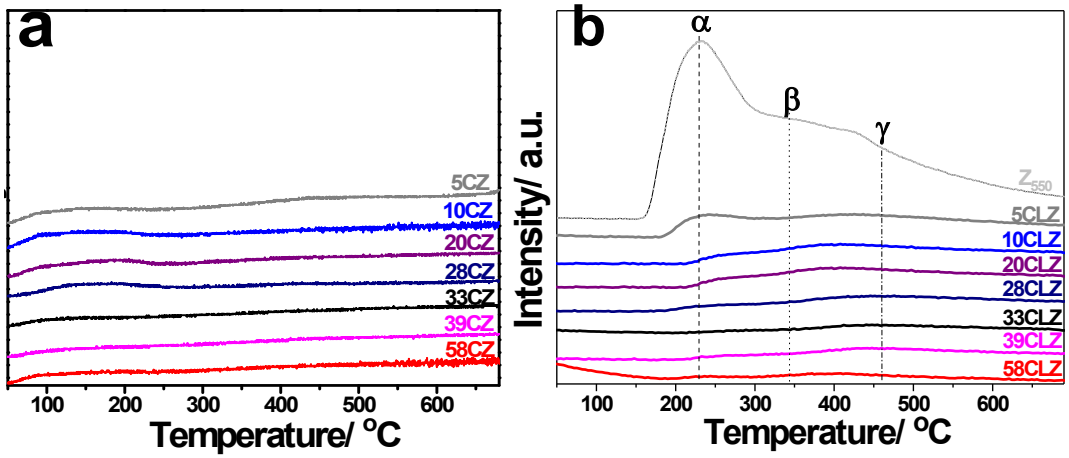

Figure S3. NH_3−TPD profiles of as-prepared catalysts (a: *w*CZ; b: *w*CLZ and standard ZrO_2).

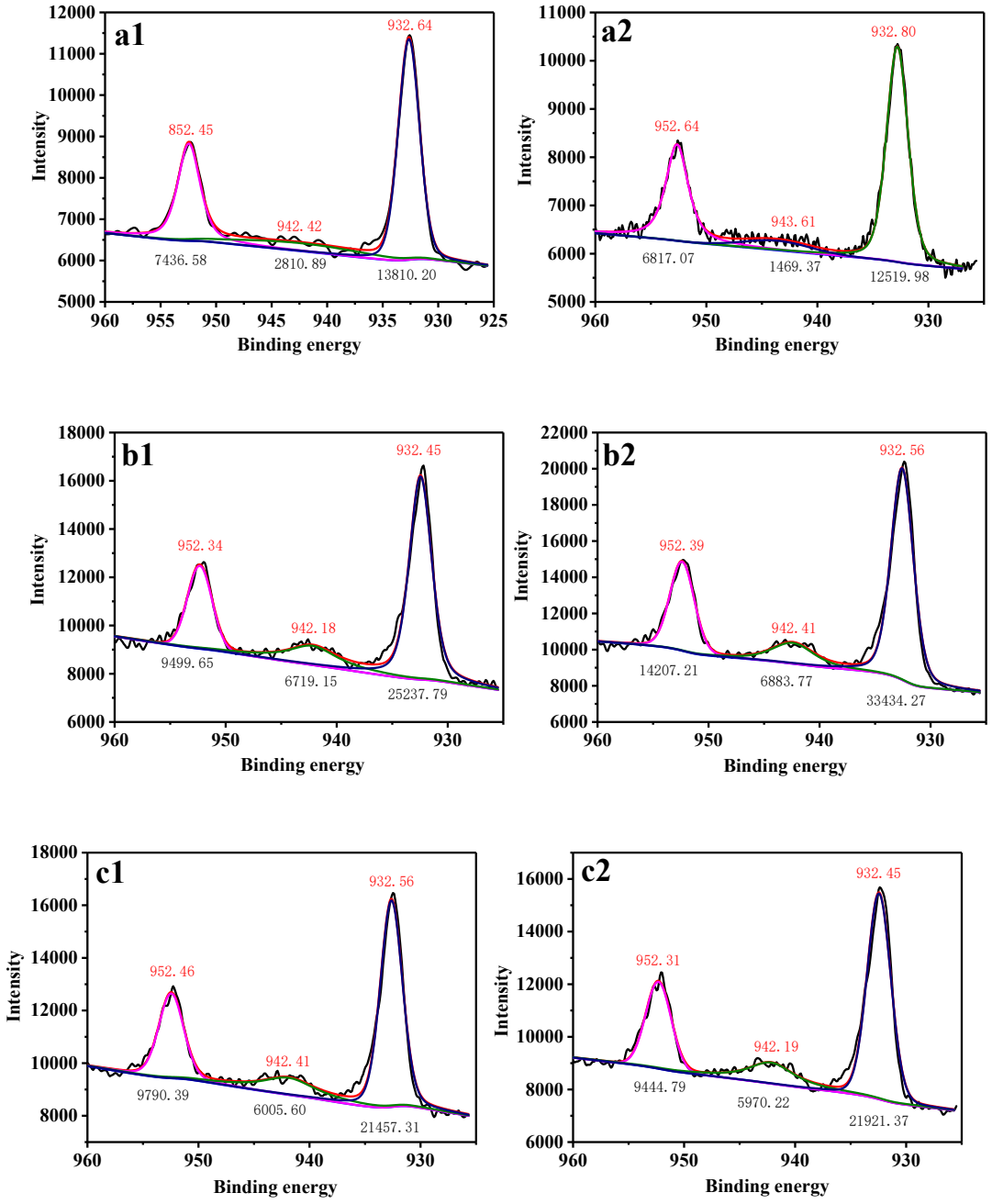

Figure S4. Cu 2p spectra of reduced catalysts (a1: 5CZ; a2: 5CLZ; b1: 33CZ; b2: 33CLZ; c1: 39CZ; c2: 39CLZ).

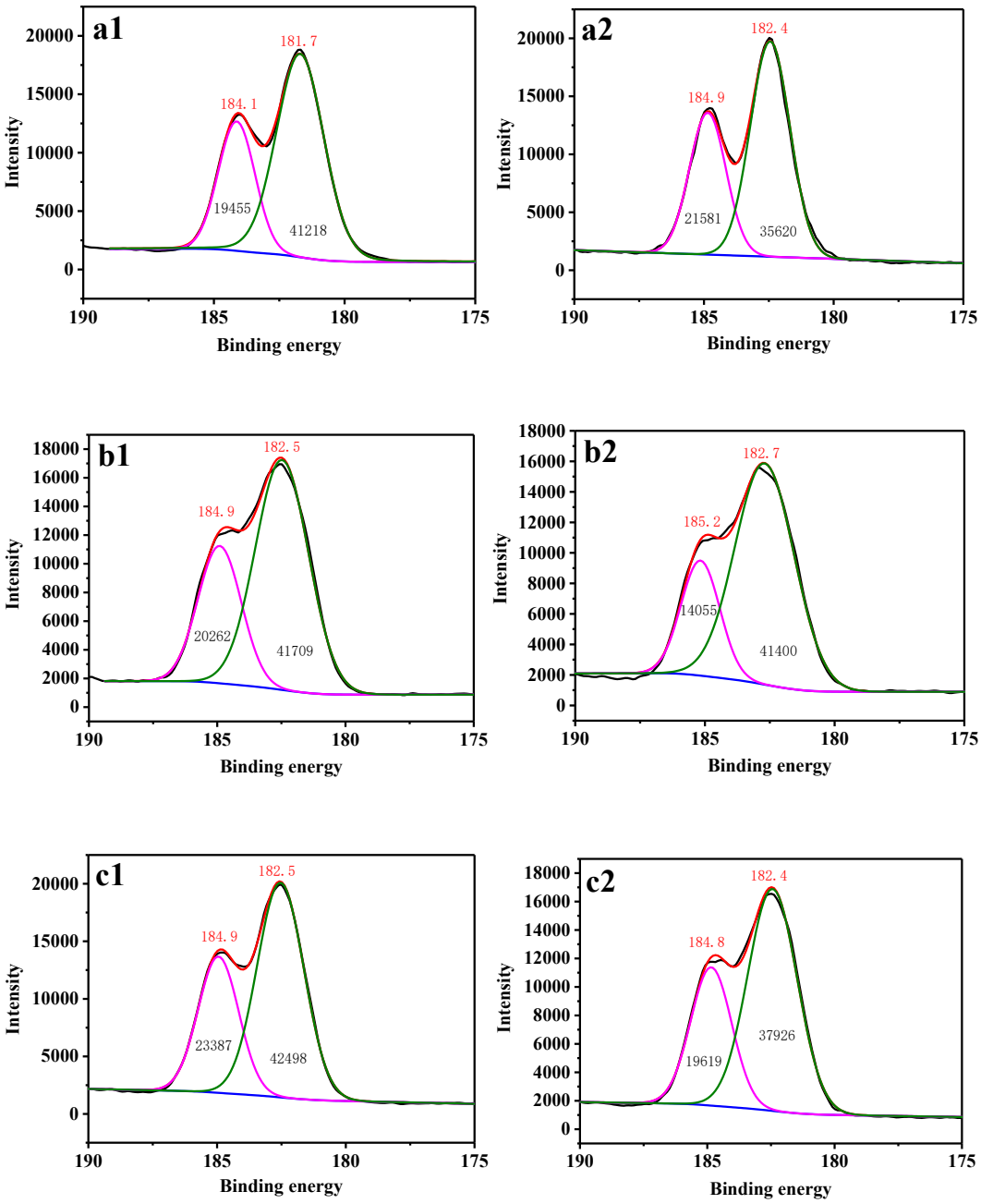

Figure S5. Zr 3d spectra of reduced catalysts (a1: 5CZ; a2: 5CLZ; b1: 33CZ; b2: 33CLZ; c1: 39CZ; c2: 39CLZ).

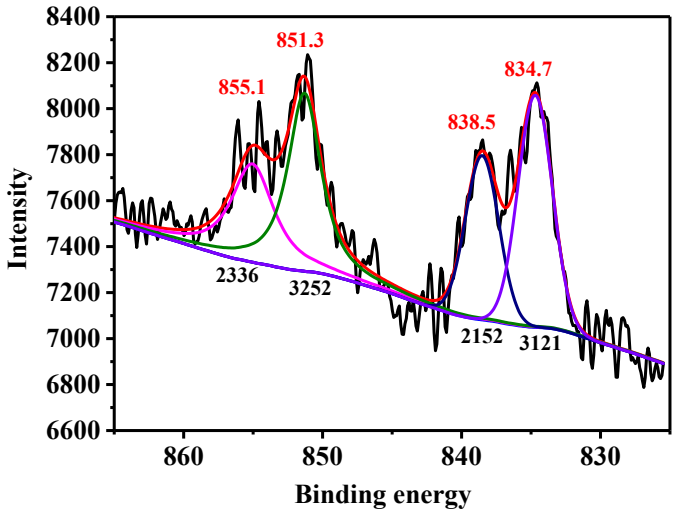

Figure S6. La 3d spectra of reduced 33CLZ catalysts.