Supporting Information

Elucidation of Ce/Zr ratio effects on the physical properties and catalytic performance of $CuO_x/Ce_yZr_{1-y}O_2$ catalysts

Mohammed Sifat[1], Michal Luchowski[1], Amol Pophali[1], Wenhui Jiang[1], Yunfan Lu[1], Byeongseok Kim[2], Gihan Kwon[3], Kwangsuk Yoon[4], Jihun Kim[5], Kwangjin An[5], Sang Eun Shim[2], Hocheol Song[4], Taejin Kim[1,*]

[1] Materials Science and Chemical Engineering Department, Stony Brook University, Stony Brook, NY, 11794, U.S.A
[2] Department of Chemistry and Chemical Engineering, Education and Research Center for Smart Energy and Materials, Inha University, Incheon, 22212, South Korea
[3] National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY 11973, U.S.A
[4] Department of Earth Resources and Environmental Engineering, Hanyang University, Seoul 04763, Republic of Korea
[5] School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea

*Corresponding author

Prof. Taejin Kim; Email: taejin.kim@stonybrook.edu

Visible Raman spectroscopy:

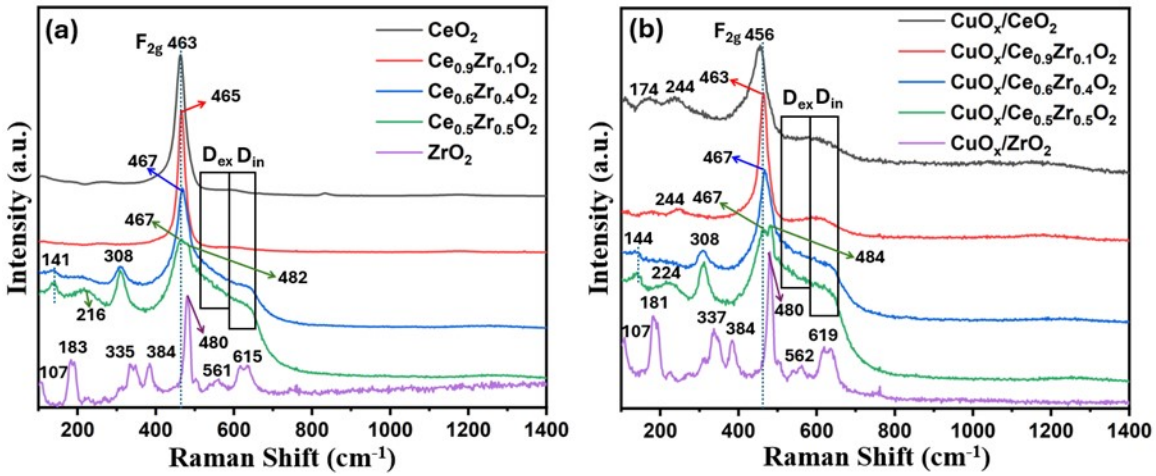

Figure S1. Visible (λ = 532 nm) Raman spectroscopy for (a) $Ce_yZr_{1-y}O_2$ (y = 1.0, 0.9, 0.6, 0.5, 0.0) supports; and (b) $CuO_x/Ce_yZr_{1-y}O_2$ (y = 1.0, 0.9, 0.6, 0.5, 0.0) catalysts.

XRD calculations:

To understand the crystalline structure of the supports and synthesized catalysts, XRD analysis was performed. The crystallite size and lattice parameters were calculated from the following equations:

$$Q = \frac{4 * \pi}{\lambda} * \sin\left(\frac{2\theta}{2}\right), \quad D = \frac{k * \lambda}{\beta * \cos(\theta)} \text{ (Scherrer equation)} \tag{5}$$

$$d_{hkl} = \frac{n * \lambda}{2 * sin(\theta)}, \quad a = \sqrt{h^2 + k^2 + l^2} \times d_{hkl} \tag{6}$$

where Q = collected scattered intensity, λ = wavelength of x-ray, θ = diffraction angle, D = average crystallite size, k = constant or shape factor (set at 0.9), β = full width at half maximum (FWHM) of the peak, d_{hkl} = d spacing of the crystal layers, n = constant (set at 1.0), and a = lattice parameter.

CO oxidation reaction tests performed on $CuO_x/Ce_yZr_{1-y}O_2$ (y = 1.0, 0.9, 0.6, 0.5, 0.0) catalysts:

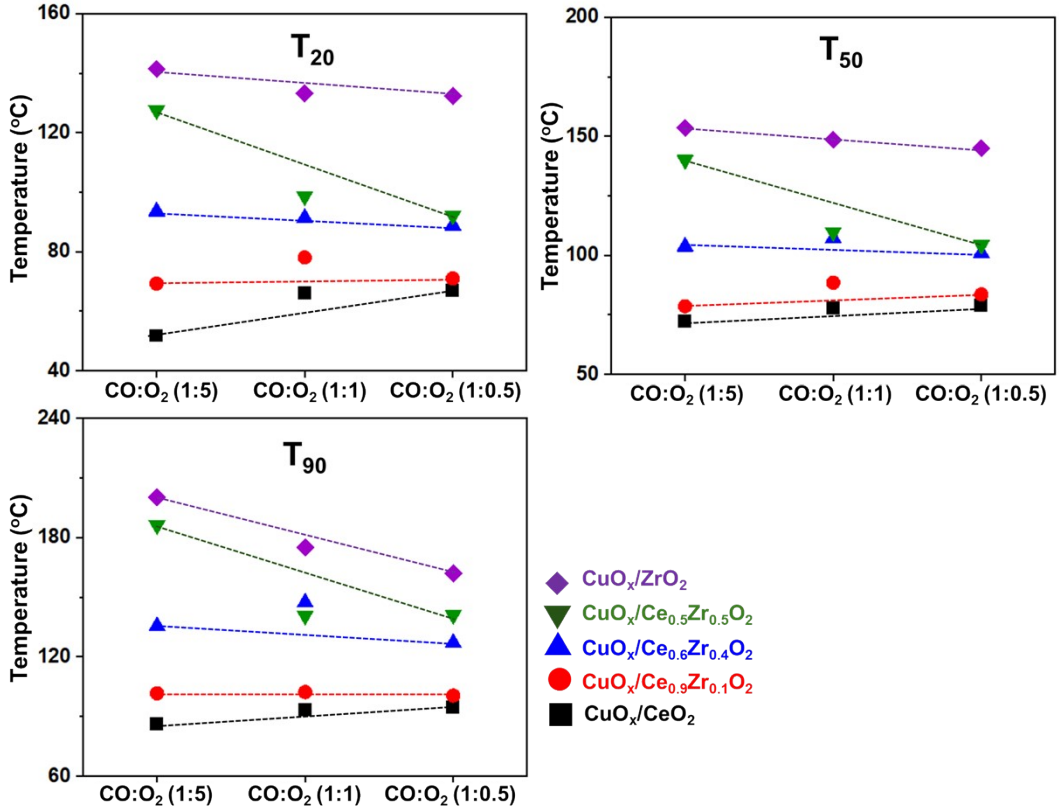

Figure S2. T_{20}, T_{50}, and T_{90} for $CuO_x/Ce_yZr_{1-y}O_2$ synthesized catalysts with varied $CO:O_2$ ratio.

Table S1. T_{20}, T_{50}, and T_{90} for $CuO_x/Ce_yZr_{1-y}O_2$ catalysts.

Sample	$CO:O_2$ (1:5) (°C)			$CO:O_2$ (1:1) (°C)			$CO:O_2$ (1:0.5) (°C)		
	T_{20}	T_{50}	T_{90}	T_{20}	T_{50}	T_{90}	T_{20}	T_{50}	T_{90}
CuO_x/CeO_2	51.8	72.4	86.0	66.2	77.7	93.2	67.0	78.9	94.7
$CuO_x/Ce_{0.9}Zr_{0.1}O_2$	69.3	78.6	101.7	78.1	88.5	102.3	71.0	83.6	100.5
$CuO_x/Ce_{0.6}Zr_{0.4}O_2$	93.6	103.7	135.4	91.4	107.2	147.3	88.8	100.9	127.0
$CuO_x/Ce_{0.5}Zr_{0.5}O_2$	127.6	140.1	186.2	98.7	109.8	140.7	92.2	104.3	141.0

CuO_x/ZrO_2	141.5	153.6	200.3	133.3	148.6	175.1	132.4	145.1	162.0