Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

High Temperature-Water Gas Shift on Ni-Cu/CeO_2 Catalysts: Effect of Ceria Nano-Crystal Size on Carboxylate Formation

*E.T Saw, U. Oemar, M.L. Ang, K. Hidajat and S. Kawi**

Department of Chemical and Bio-molecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117585

*To whom correspondence should be addressed

Address: Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117585

Telephone: (65) 6516 6312; Fax: (65) 6779 1936

E-Mail address: chekawis@nus.edu.sg. (S. Kawi)

SUPPORTING INFORMATION

(i) Particle Size Distribution of CeO_2 (1)

Figure S1 displays the particle size distribution of CeO_2 (1) prepared using the concentration of cerium-nitrate as catalyst precursors of 13.5mM and 2.25g of PVP360K dissolved in deionized water and placed into oven at 140°C for 12 hours. Calcination in air at 700°C for 2hours and the sizes are ranged from 150 to 350nm where the high frequencies of particles sizes are shown within 275-300 nm and the average ceria particle size is 284 nm.

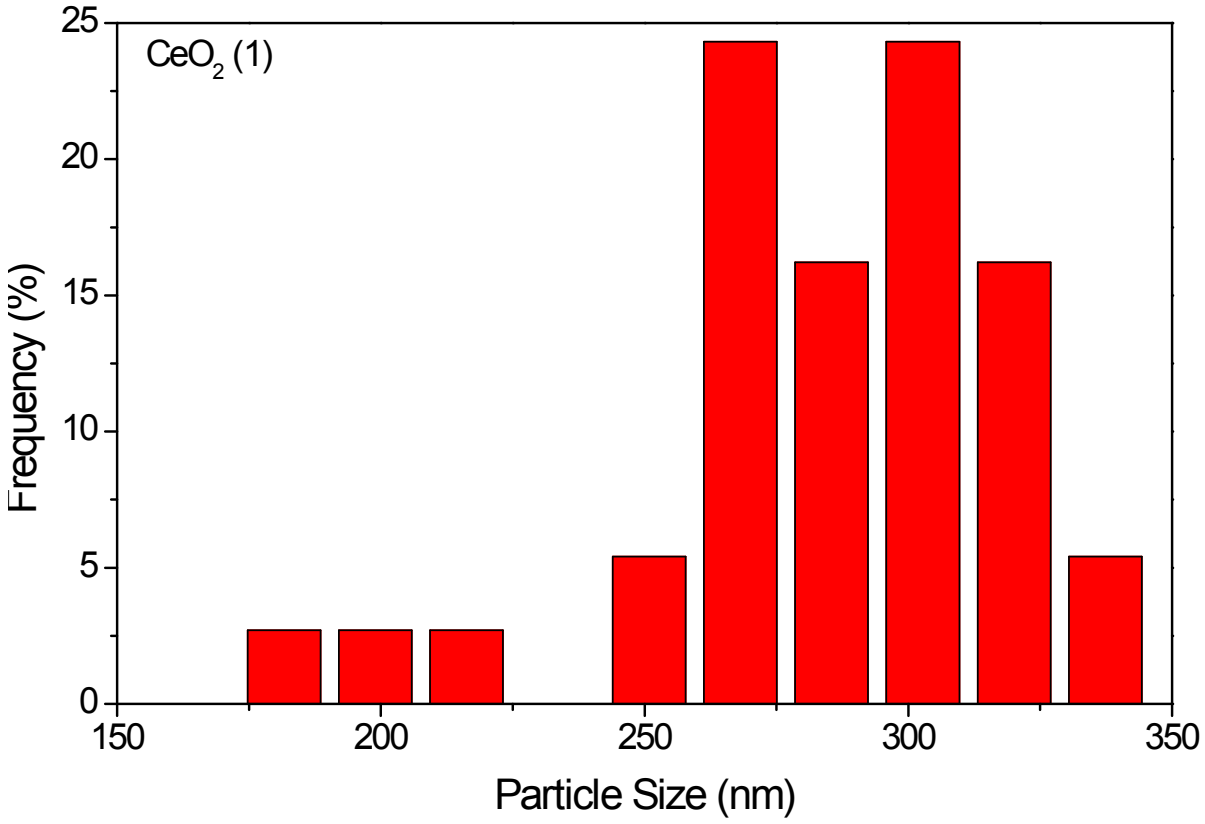

Figure S1. Particle Size Distribution of CeO_2 (1)

(ii) Particle Size Distribution of CeO_2 (2)

Figure S2 displays the particle size distribution of CeO_2 (2) prepared using the concentration of cerium-nitrate as catalyst precursors of 22.5mM and 2.25g of PVP360K dissolved in deionized water and put into 140°C for 48hours. Calcination in air at 700°C for 2hours and the sizes are ranged from 400 to 800nm where the high frequencies of particle sizes are shown within 500-600 nm and the average ceria particle size is 550 nm.

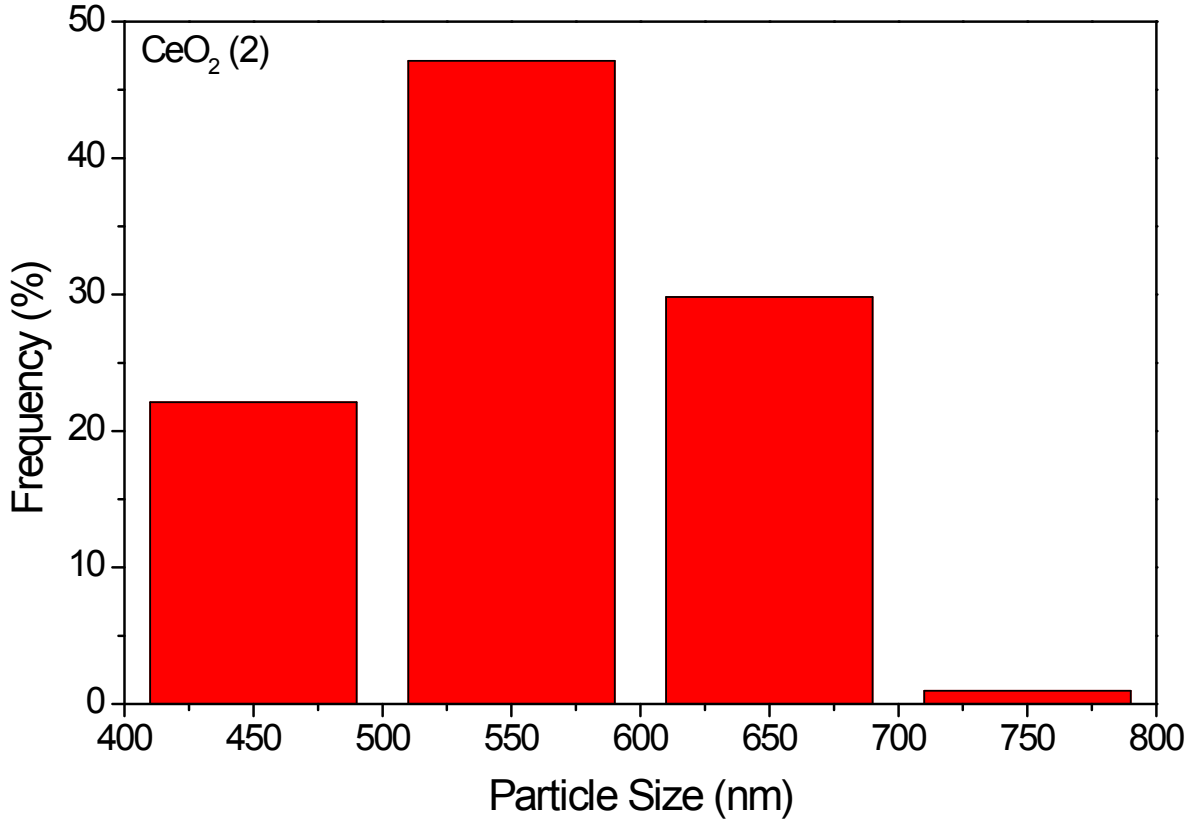

Figure S2. Particle Size Distribution of CeO_2 (2)

(iii) Particle Size Distribution of CeO_2 (3)

Figure S3 displays the particle size distribution of CeO_2 (2) prepared using the concentration of cerium-nitrate as catalyst precursors of 22.5mM and 2.25g of PVP360K dissolved in deionized water and put into 140°C for 96 hours. Calcination in air at 700°C for 2hours and the sizes are ranged from 800 to 1200nm where the high frequency of particle sizes are shown within 900-1000nm and the average ceria particle size is 946 nm.

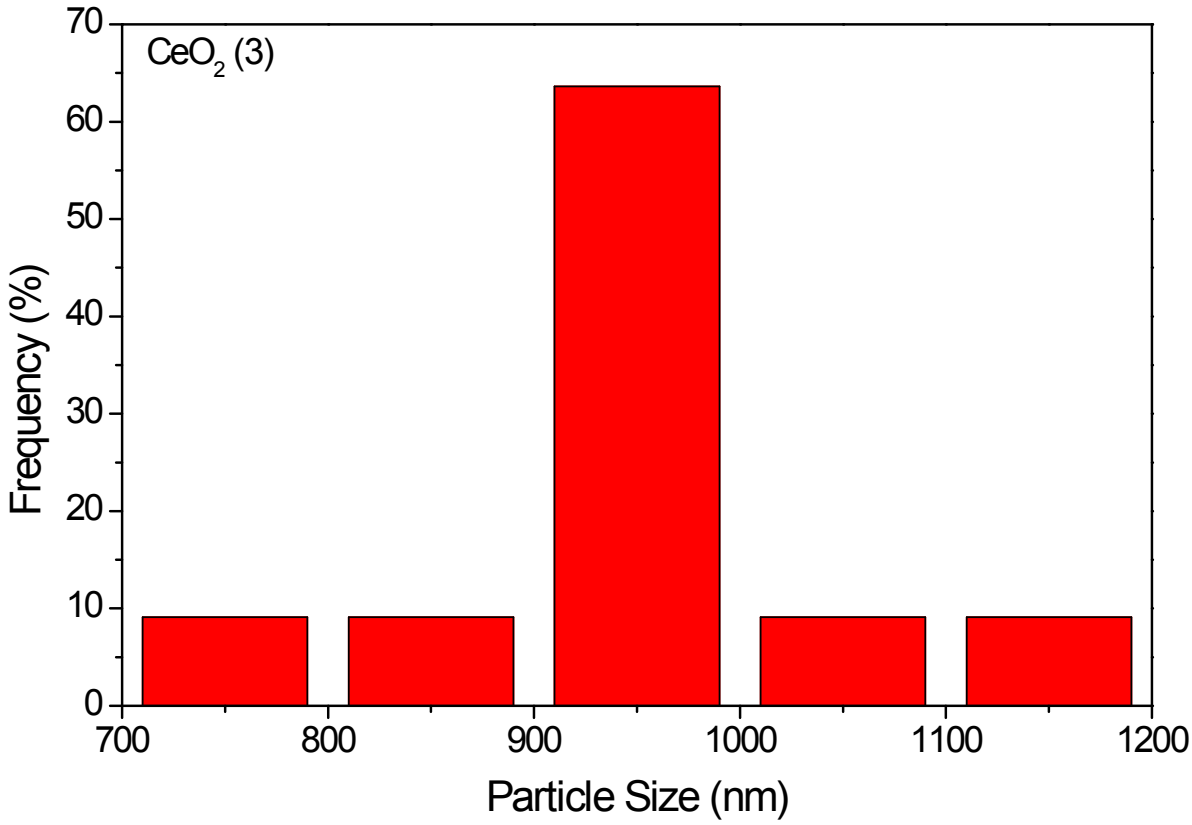

Figure S3. Particle Size Distribution of CeO_2 (3)

(iv) N_2O decomposition over reduced CeO_2 (1)

Figure S4 displays the TPR_1 and TPR_2 profiles obtained during N_2O decomposition technique. TPR_1 is carried out freshly calcined CeO_2 (1) support upto 700°C for 1 h. Whereas, TPR_2 is carried out after N_2O pulse at 80°C. The amount of H_2 consumed during TPR_2 is 14.08 µmol/g. This result shows about 0.8% in 11.4% of 5Ni-5Cu/CeO2 (1) catalyst's dispersion is obtained from CeO_2 (1) support.

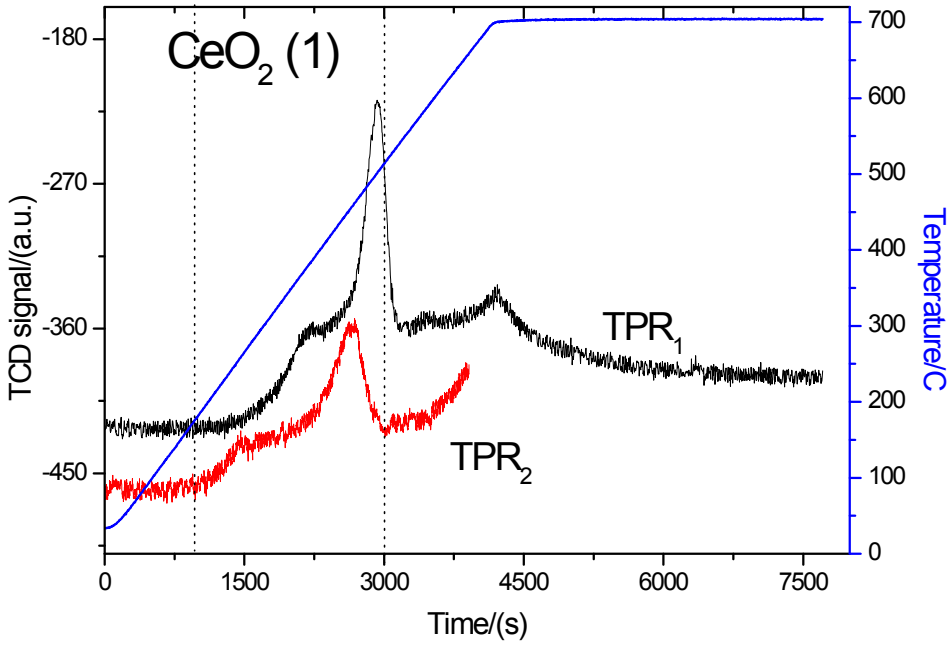

Figure S4. H_2-TPR's during N_2O decomposition technique over reduced CeO_2 (1)

(v) N_2O decomposition over reduced CeO_2 (2)

Figure S5 displays the TPR_1 and TPR_2 profiles obtained during N_2O decomposition technique. TPR_1 is carried out freshly calcined CeO_2 (2) support upto 700°C for 1 h. Whereas, TPR_2 is carried out after N_2O pulse at 80°C. The amount of H_2 consumed during TPR_2 is 3.93 µmol/g. This result shows about 0.2% in 12.3% of 5Ni-5Cu/CeO_2 (2) catalyst's dispersion is obtained from CeO_2 (2) support.

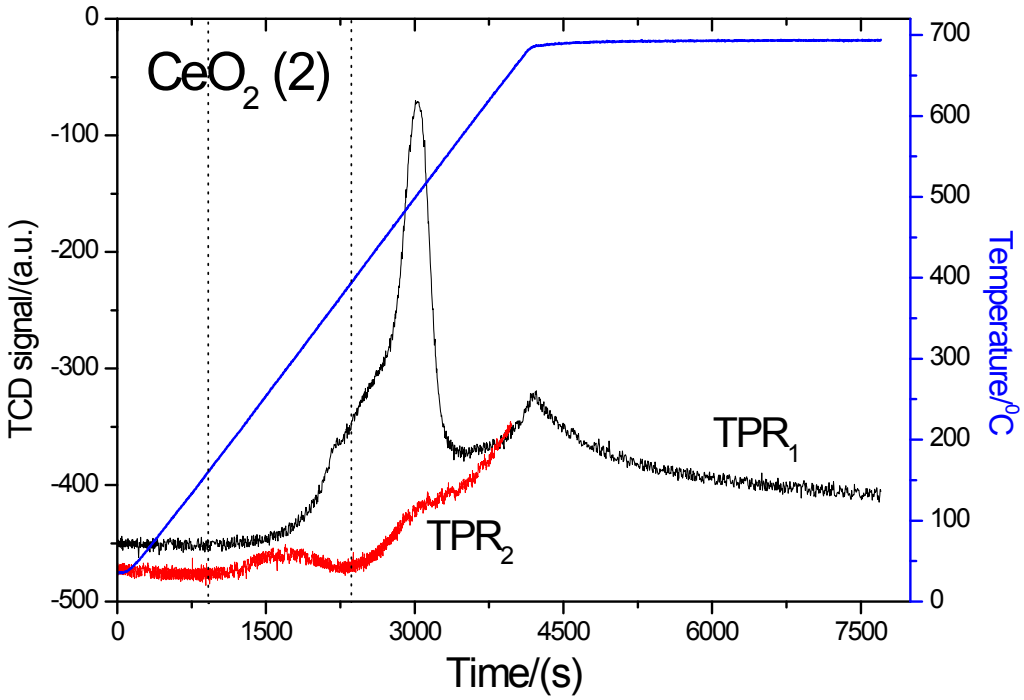

Figure S5. H_2-TPR's during N_2O decomposition technique over reduced CeO_2 (2)

(vi) N_2O decomposition over reduced CeO_2 (3)

Figure S6 displays the TPR_1 and TPR_2 profiles obtained during N_2O decomposition technique. TPR_1 is carried out freshly calcined CeO_2 (3) support upto 700°C for 1 h. Whereas, TPR_2 is carried out after N_2O pulse at 80°C. The amount of H_2 consumed during TPR_2 is 8.23 µmol/g. This result shows about 0.4% in 15.1% of 5Ni-5Cu/CeO_2 (3) catalyst's dispersion is obtained from CeO_2 (3) support.

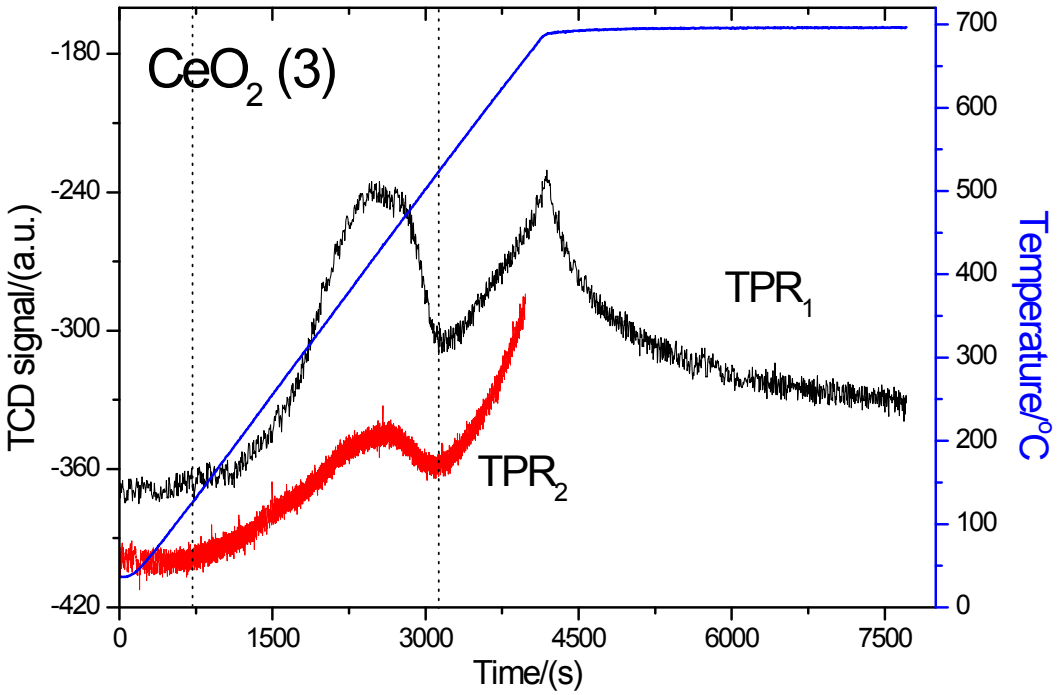

Figure S6. H_2-TPR's during N_2O decomposition technique over reduced CeO_2 (3)

(vii) Bimetallic Particle Size of supported 5Ni5Cu/CeO_2 (1)

Figure S7 displays the particle size distribution of Ni-Cu bimetallic particle size prepared after reduction of 5Ni5Cu/CeO_2 (1) at 450°C. The bimetallic sizes are ranged from 10-35 nm where the high frequencies of particle sizes are shown within 15-25 nm and the average of bimetallic particle size is 22.4nm.

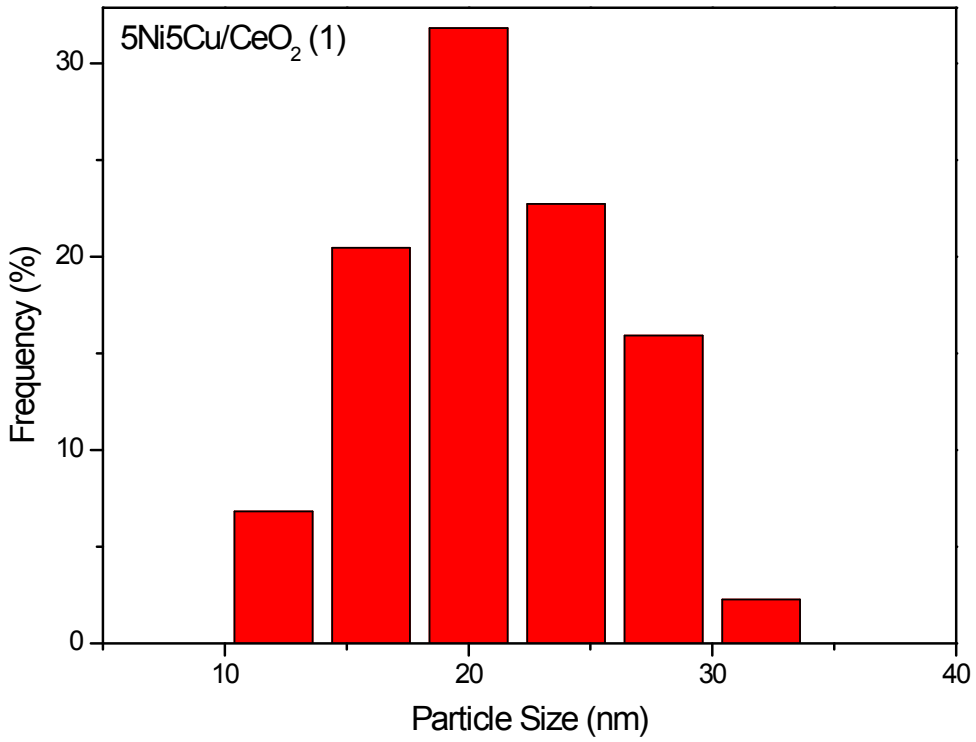

Figure S7. Particle Size Distribution of 5Ni5Cu/CeO_2 (1)

(viii) Bimetallic Particle Size of supported 5Ni5Cu/CeO_2 (2)

Figure S8 displays the particle size distribution of Ni-Cu bimetallic particle size prepared after reduction of 5Ni5Cu/CeO_2 (2) at 450°C. The bimetallic sizes are ranged from 10-60 nm where the high frequencies of particle sizes are shown within 20-35 nm and the average particle size is 29.4 nm.

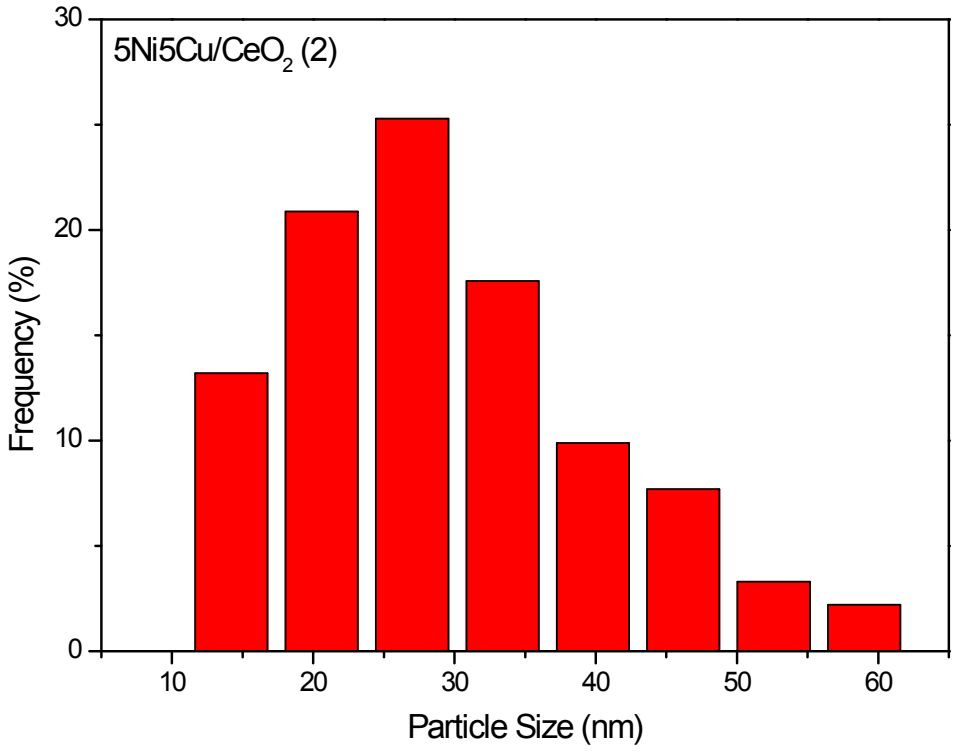

Figure S8. Particle Size Distribution of 5Ni5Cu/CeO_2 (2)

(ix) Bimetallic Particle Size of supported 5Ni5Cu/CeO_2 (3)

Figure S9 displays the particle size distribution of Ni-Cu bimetallic particle size prepared after reduction of 5Ni5Cu/CeO_2 (3) at 450°C. The bimetallic sizes are ranged from where the high frequencies of particle sizes are shown within 20-35 nm and the average particle size is 28.3 nm.

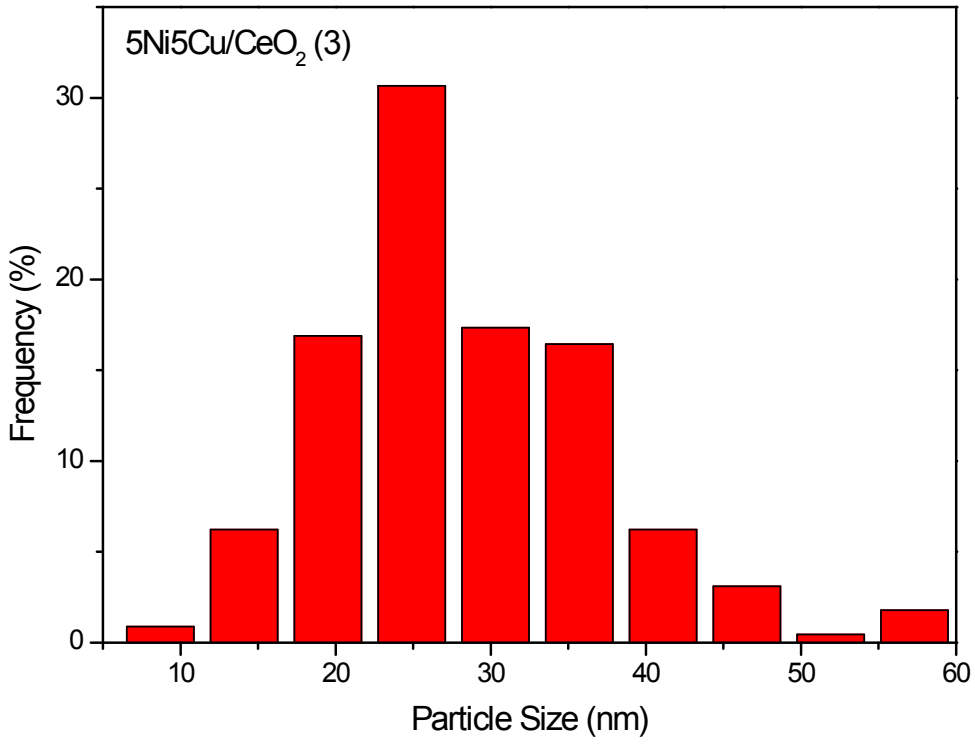

Figure S9. Particle Size Distribution of 5Ni5Cu/CeO_2 (3)

(x) Bimetallic Particle Size of spent catalyst (5Ni5Cu/CeO_2 (3)) for 30 hours of catalytic stability test

Figure S10 displays the particle size distribution of Ni-Cu bimetallic particle size prepared after the stability test of 5Ni5Cu/CeO_2 (3) at 450°C. The bimetallic sizes are ranged from 20-60 nm where the high frequencies of particle sizes are shown within 25-35 nm and the average of the bimetallic particle size is 33.9 nm.

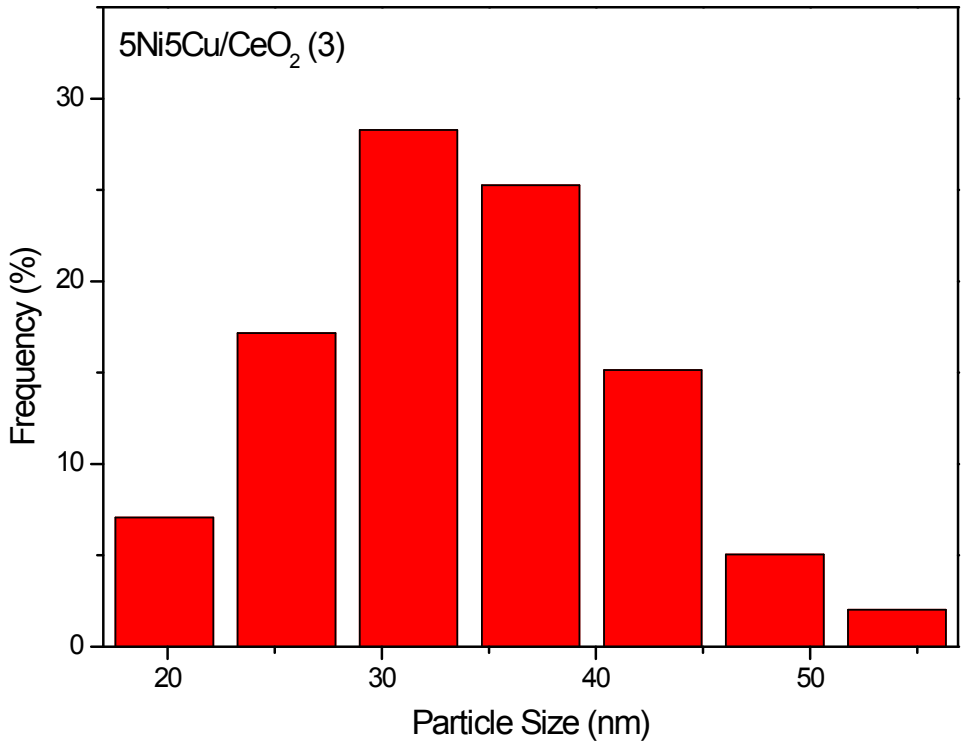

Figure S10. Particle Size Distribution of spent 5Ni5Cu/CeO_2 (3)