

Enhanced Cyclopentanone Yield from Furfural Hydrogenation: Promotional Effect of Surface Silanols on Ni-Cu/m-silica Catalyst

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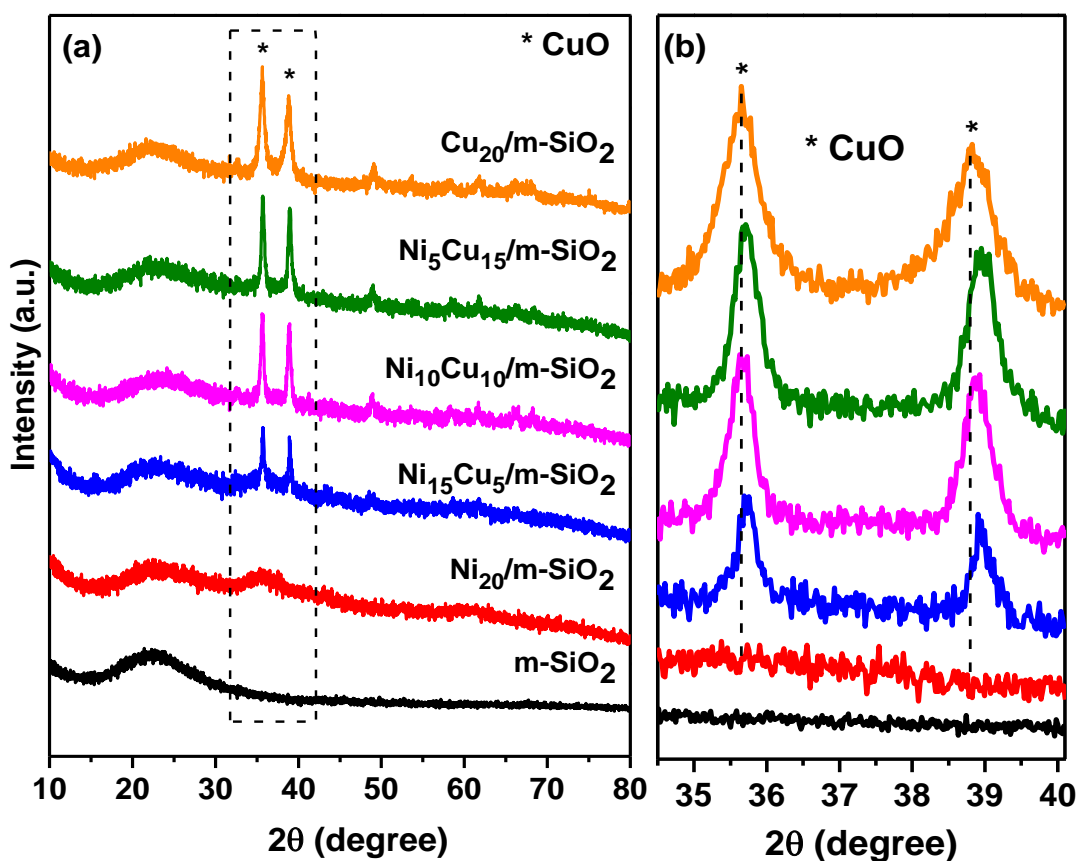


Figure S1. (a) XRD patterns of calcined pure m-SiO₂ and Ni_xCu_y/m-SiO₂ (total metal loading fixed at 20 wt.% with varied relative Ni and Cu loading) and (b) expanded view of XRD patterns in 2θ from 34° to 40°.

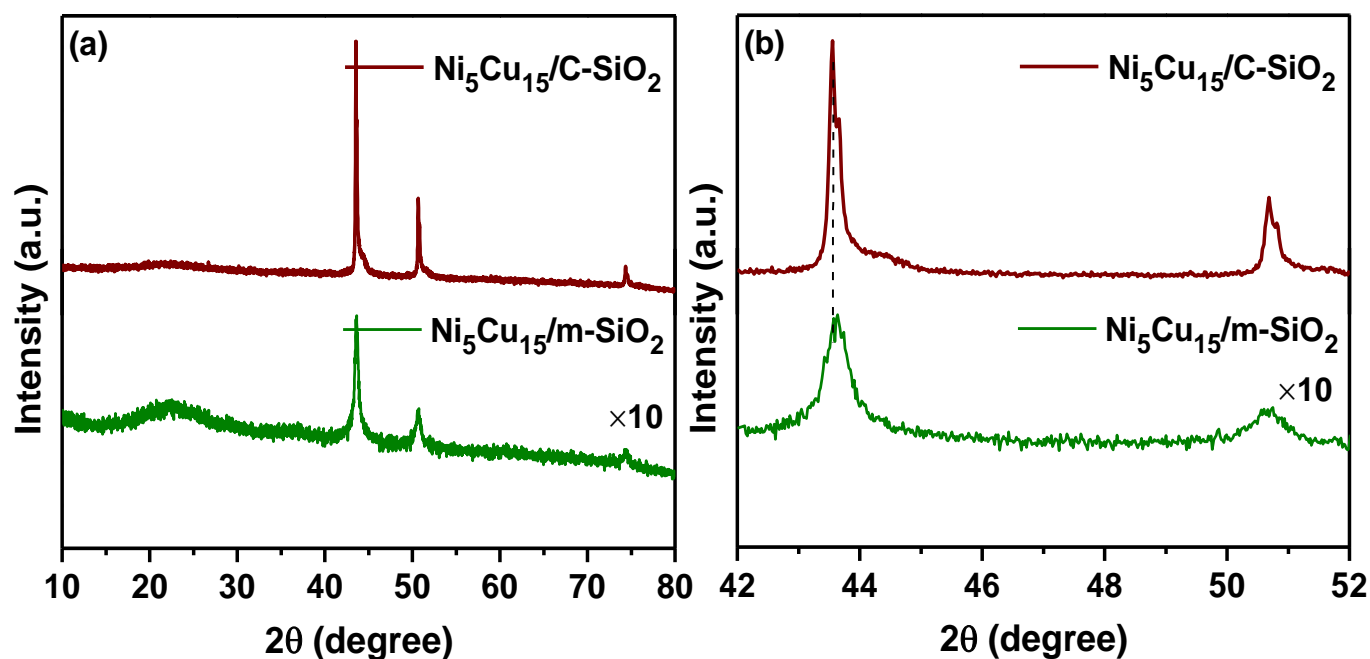


Figure S2. (a) XRD patterns of reduced $\text{Ni}_5\text{Cu}_{15}/\text{m-SiO}_2$ and $\text{Ni}_5\text{Cu}_{15}/\text{C-SiO}_2$ catalysts and (b) expanded view of XRD patterns in 2θ from 42° to 52° .

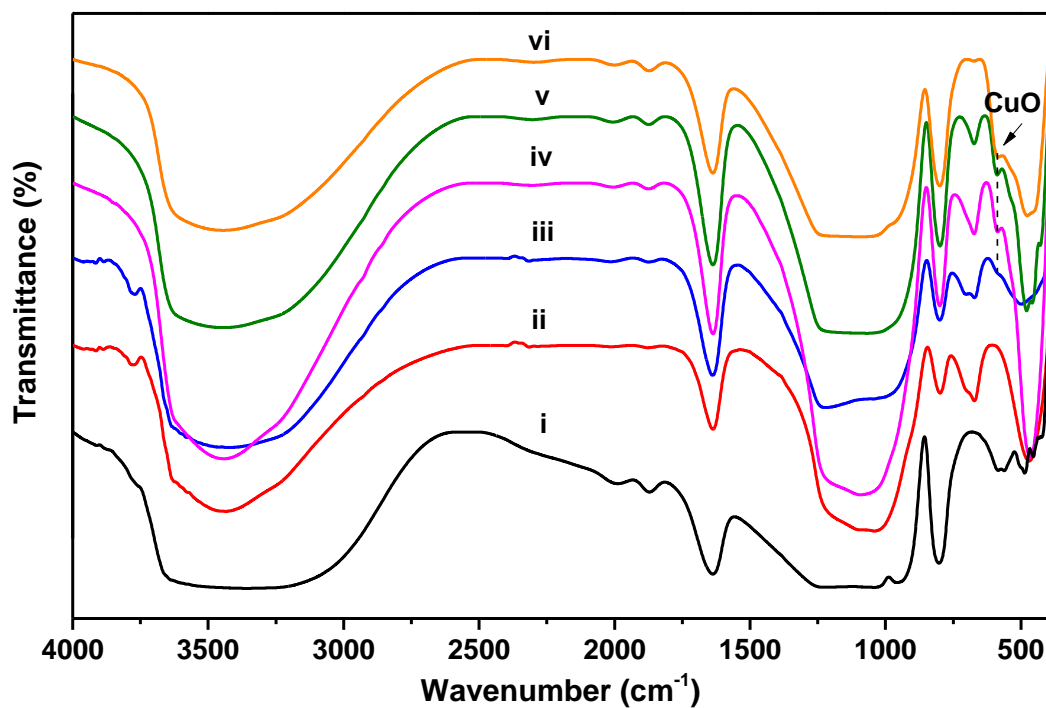


Figure S3. FTIR spectra of calcined (i) pure m-SiO_2 , (ii) $\text{Ni}_{20}/\text{m-SiO}_2$, (iii) $\text{Ni}_{15}\text{Cu}_5/\text{m-SiO}_2$, (iv) $\text{Ni}_{10}\text{Cu}_{10}/\text{m-SiO}_2$, (v) $\text{Ni}_5\text{Cu}_{15}/\text{m-SiO}_2$, and (vi) $\text{Cu}_{20}/\text{m-SiO}_2$ catalysts.

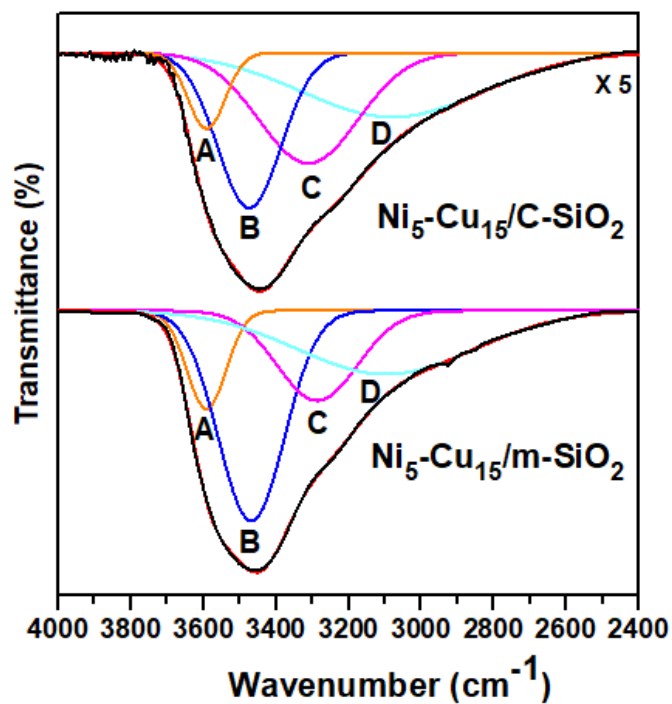


Figure S4. FTIR of reduced catalysts.

Table S1. Characteristic spectra peaks of FTIR.

S.No	Catalyst	A+B (%)	C+D (%)
1	Ni ₅ -Cu ₁₅ /m-SiO ₂	49	51
2	Ni ₅ -Cu ₁₅ /C-SiO ₂	36	64

FT-IR spectra of between 3400-3600 cm⁻¹ assigned to mono hydrogen bonded silanols (A+B) and 3200 cm⁻¹ corresponding to the poly-hydrogen bonded silanols (C+D) [53].

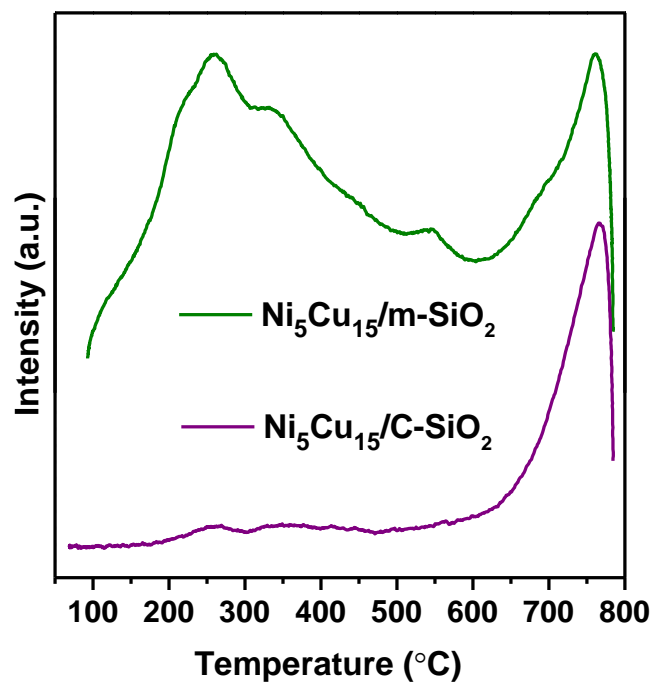


Figure S5. NH_3 -TPD of $\text{Ni}_5\text{Cu}_{15}/\text{m-SiO}_2$ and $\text{Ni}_5\text{Cu}_{15}/\text{C-SiO}_2$.

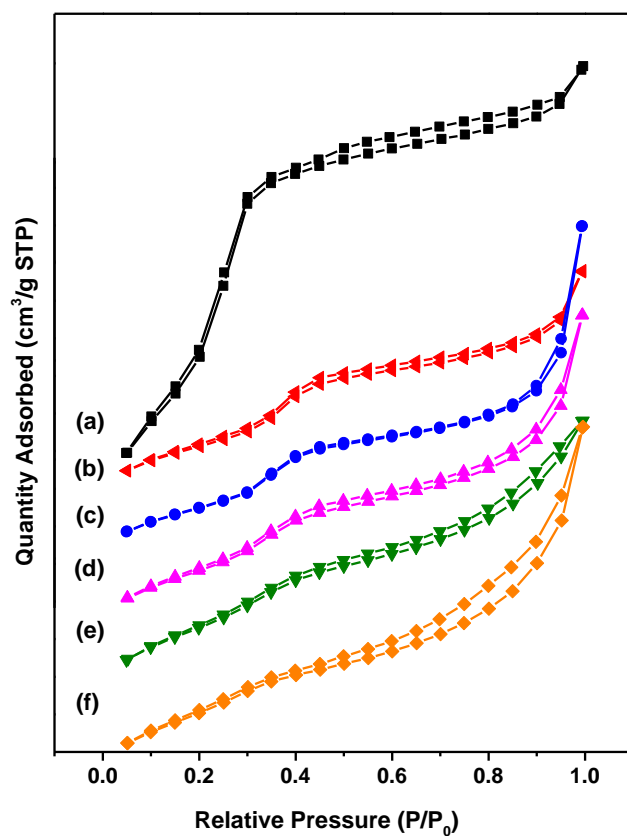


Figure S6. BET of silica after metal loading on silica. (a) m-SiO_2 , (b) $\text{Ni}_{20}/\text{m-SiO}_2$, (c) $\text{Ni}_{15}\text{Cu}_5/\text{m-SiO}_2$, (d) $\text{Ni}_{10}\text{Cu}_{10}/\text{m-SiO}_2$, (e) $\text{Ni}_5\text{Cu}_{15}/\text{m-SiO}_2$, and (f) $\text{Cu}_{20}/\text{m-SiO}_2$.

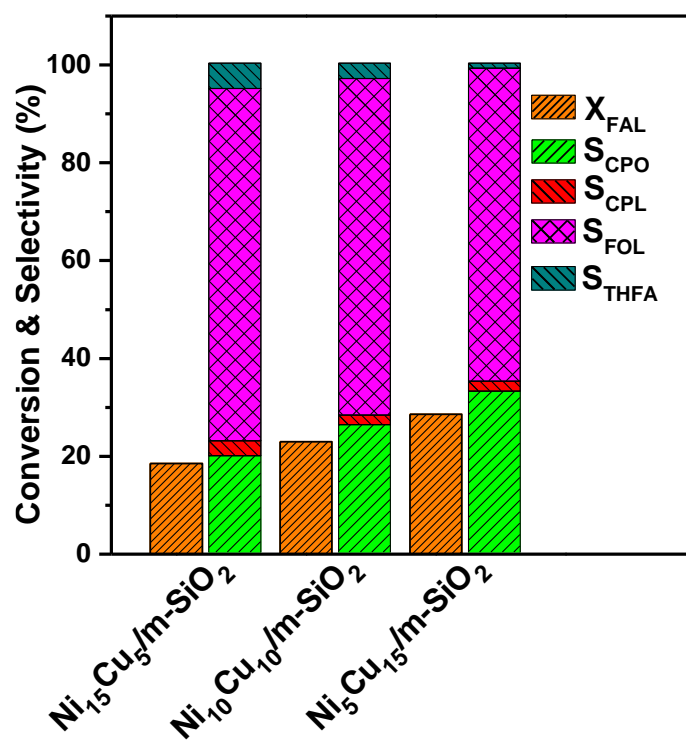


Figure S7. Catalytic performance in furfural (FAL) hydrogenation over metals supported on m-SiO₂. Reaction condition: 5.2 mmol FAL, 15 mL water, catalyst 0.05 g, 140 °C, 3 MPa H₂, and 4 h.

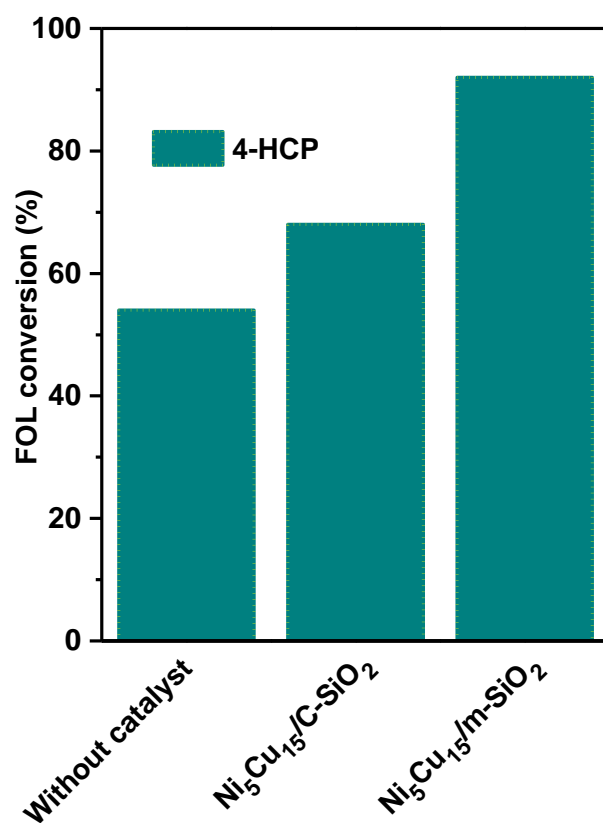


Figure S8. Rearrangement of furfuryl alcohol (FOL) to 4-hydroxy-2-cyclopentenone (4-HCP). Reaction condition: 5.2 mmol FOL, 15 mL water, reduced catalyst 0.17 g, 140 °C, 3 MPa N₂, 4 h.

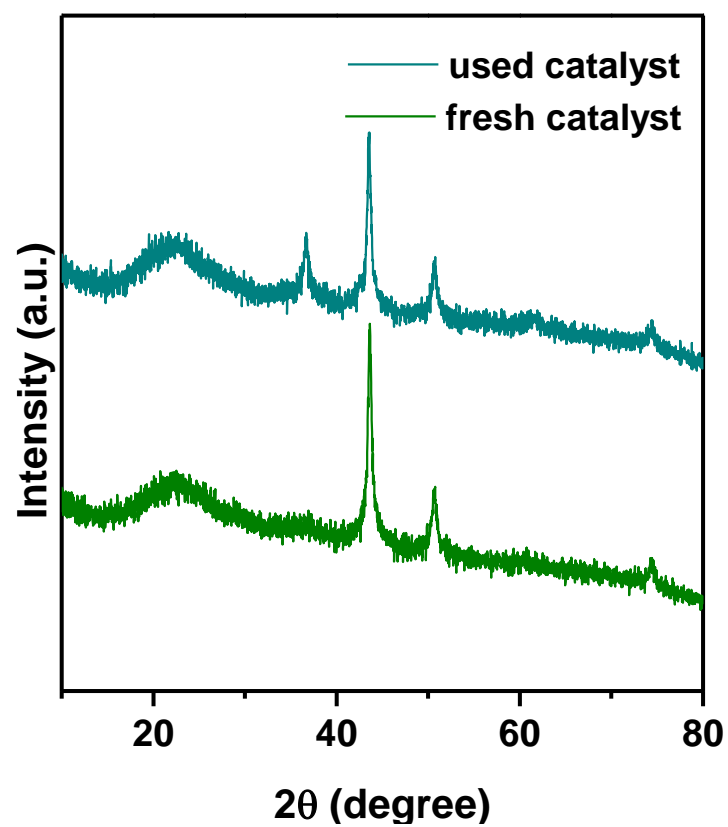


Figure S9. XRD of Ni₅Cu₁₅/m-SiO₂

Reference:

53. Hu, N.; Rao, Y.; Sun, S.; Hou, L.; Wu, P., Fan, S., Ye, B. Structural Evolution of Silica Gel and Silsesquioxane Using Thermal Curing, *Appl. Spectrosc.* 2016, 70, 1328–1338. <https://doi.org/10.1177/0003702816654063>.