

Improved CO₂ hydrogenation on Ni-ZnO/MCM-41 catalysts with the cooperative Ni and ZnO sites

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Table S1 Values of BET surface area and average pores size for Ni-ZnO/MCM-41 catalysts with different Ni loadings.

Catalyst	Surface area (m ² g ⁻¹)	Average pore size (nm) ^a
A	797	3.8
B	784	3.8
C	756	3.8
D	790	3.8
E	855	3.8

^aThe values of average pore size for different Ni-ZnO/MCM-41 catalysts were extracted from the desorption isotherms (77 K N₂) using DFT model.

Table S2 NiO particle sizes in different Ni-ZnO/MCM-41 catalysts. The values are calculated from XRD patterns of the samples using Scherrer equation.¹

Catalyst	Calculated NiO particle size (nm)
A	42.7
B	54.7
C	36.4
D	10.8
E	12.0

Table S3 Calculated dispersion from TEM images

Catalyst	Average particle size (nm)	Dispersion (%)
C	5.2	19.4
E	10.1	10.0

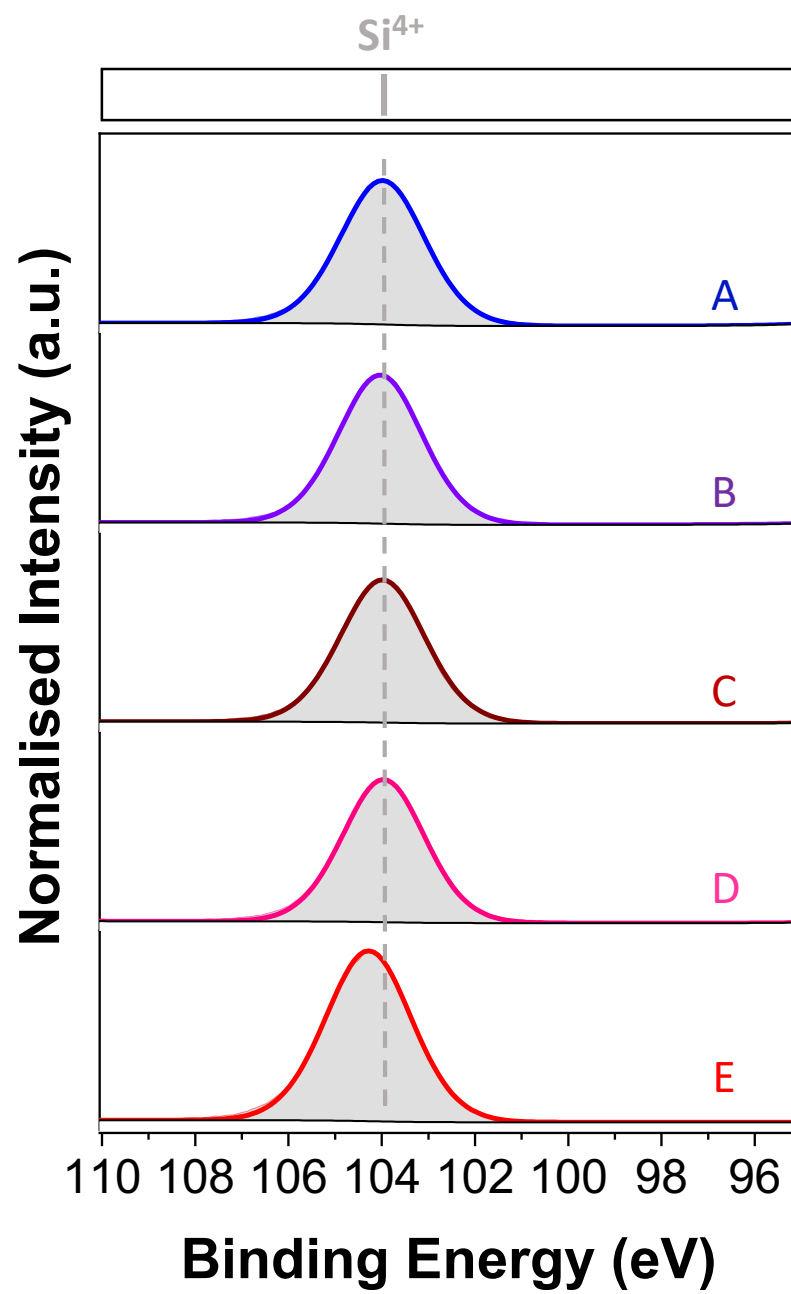


Figure S1 XPS spectrum of the Ni-ZnO/MCM-41 catalysts for silica (Si_{2p}).

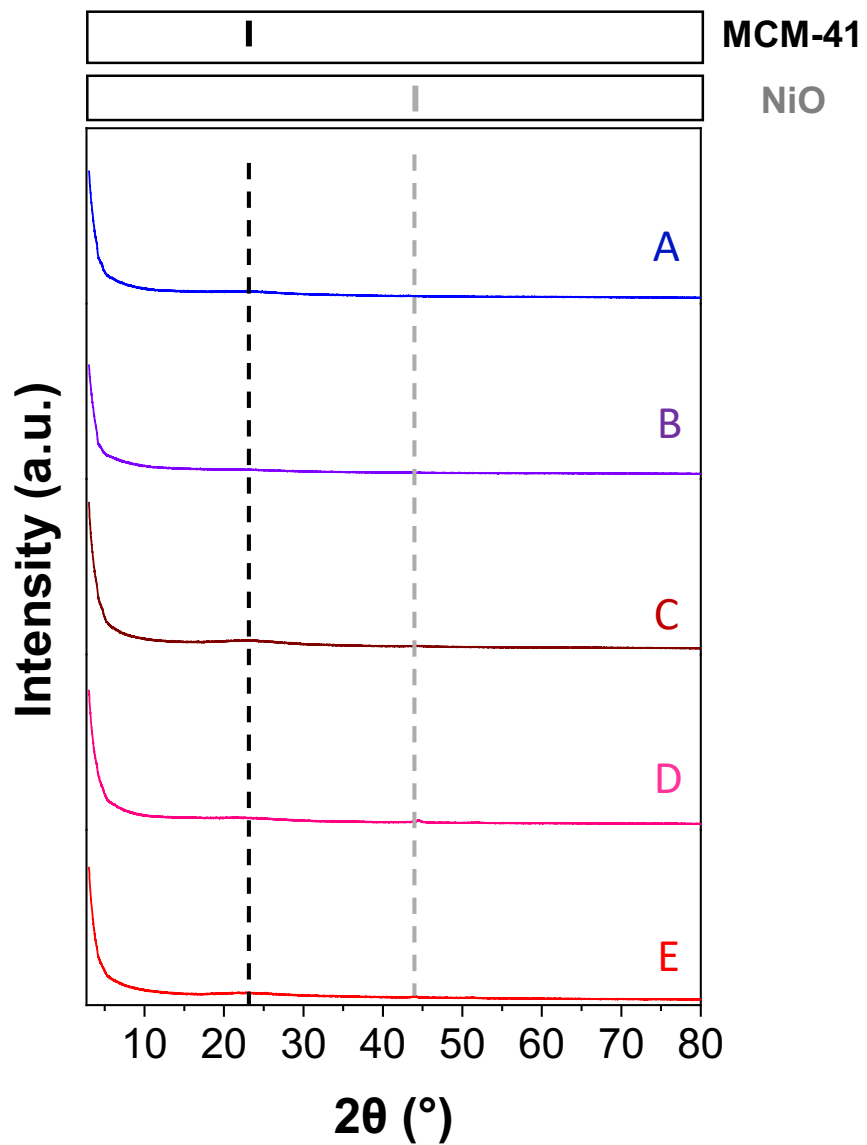


Figure S2 XRD patterns of the spent Ni-ZnO/MCM-41 catalysts. Recall from Table 1: A – 1%Ni9%Zn, B – 2.5%Ni7.5%Zn, C – 5%Ni5%Zn, D – 7.5%Ni2.5%Zn, E – 9%Ni1%Zn.

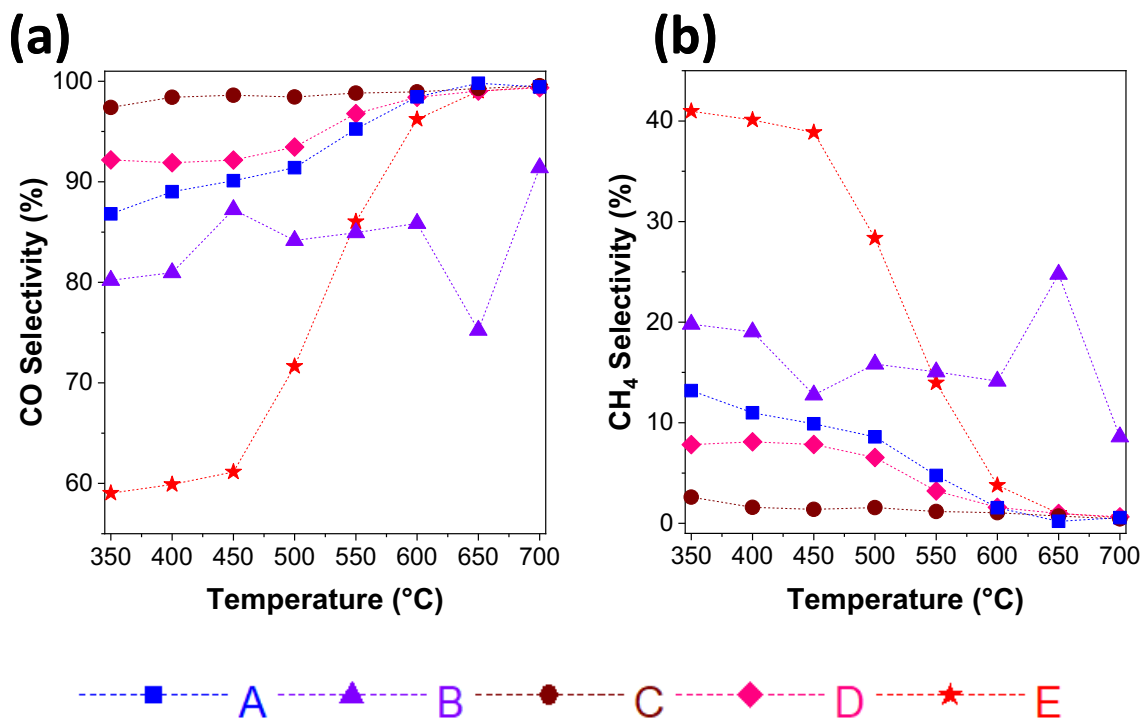


Figure S3 CH₄ (a) and CO (b) selectivity (in %) over CO₂ hydrogenation reaction. In a typical experiment, a continuous flow of CO₂/H₂/N₂ (100 mL min⁻¹, CO₂:H₂:N₂ = 6:18:76) was passed over the catalyst bed (50 mg) located within a custom-design reaction system. Data was collected over the steady state of the reaction over a temperature range of 350-700 °C.

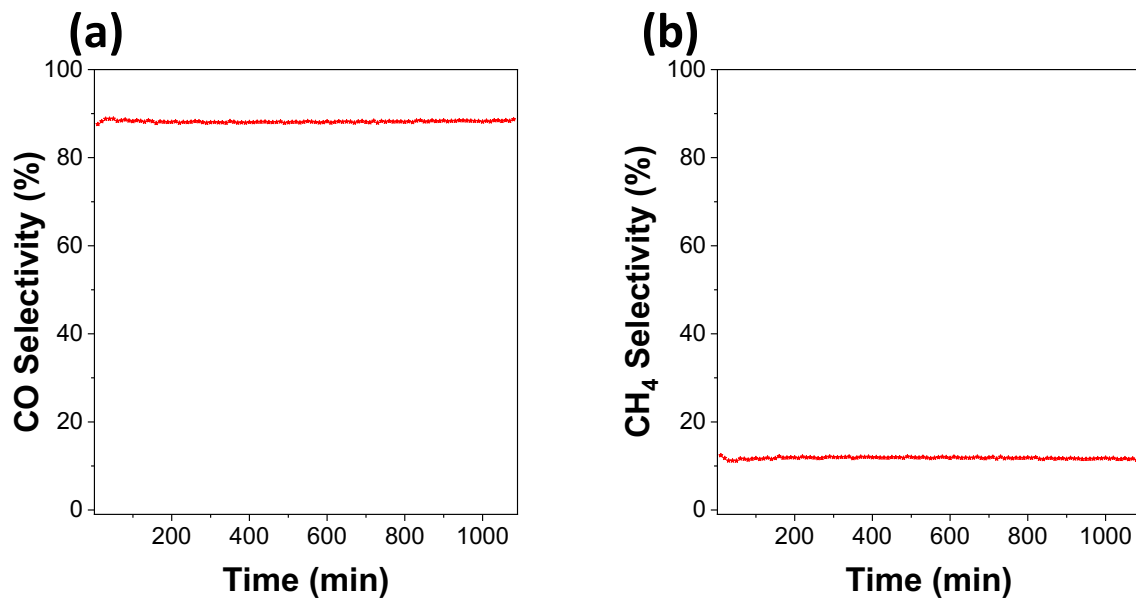


Figure S4 CH₄ (a) and CO (b) selectivity (in %) over CO₂ hydrogenation reaction for catalyst sample E. In a typical experiment, a continuous flow of CO₂/H₂/N₂ (100 mL min⁻¹, CO₂:H₂:N₂ = 6:18:76) was passed over the catalyst bed (50 mg) located within a customer-design reaction system. Data was collected over the steady state of the reaction across 24 hours.