

Supporting information for

Creation of CuO_x/ZSM-5 Zeolite Complex: Healing Defect sites, Boosting Acidic Stability and Catalytic Activity

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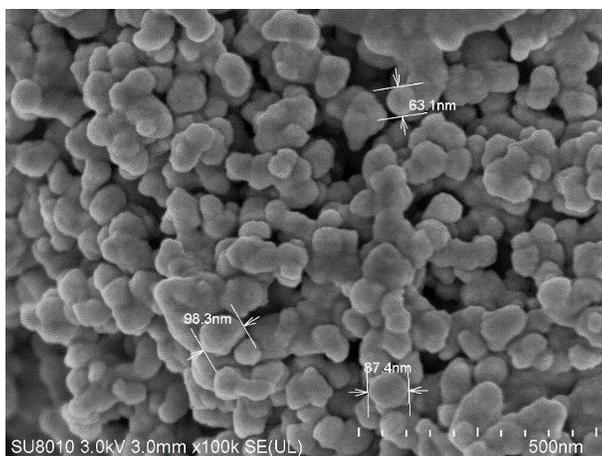


Figure S1. SEM images of the parent CuO particles, size of 60-100 nm

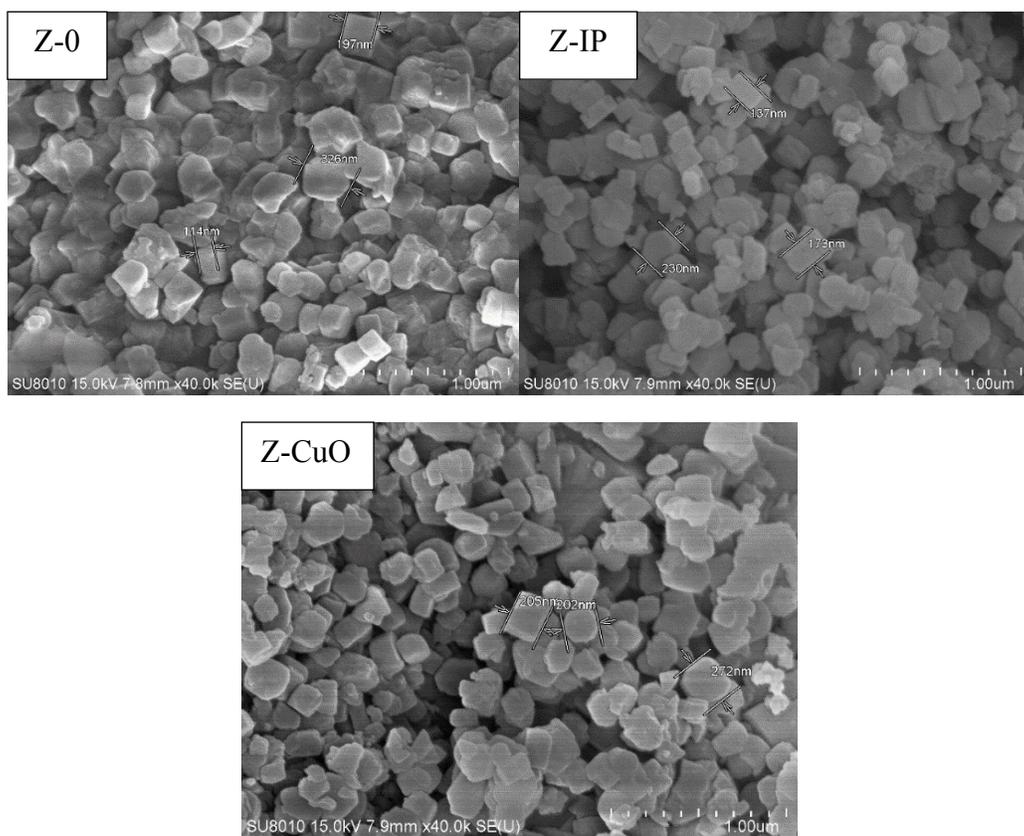


Figure S2. SEM images of Z-0 and two modified ZSM-5 samples (Z-IP and Z-CuO)

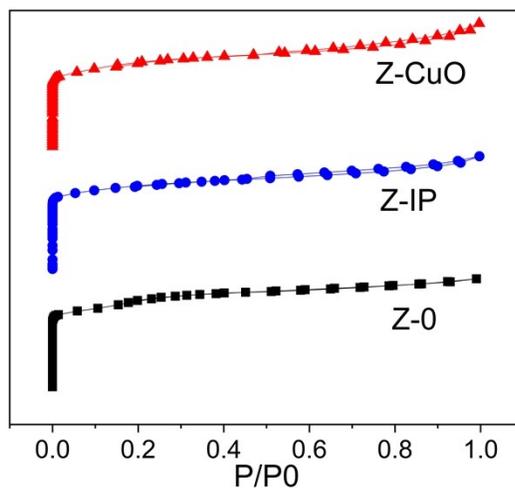


Figure S3. N₂ adsorption/desorption isotherms of Z-0 and two modified ZSM-5 samples (Z-IP and Z-CuO)

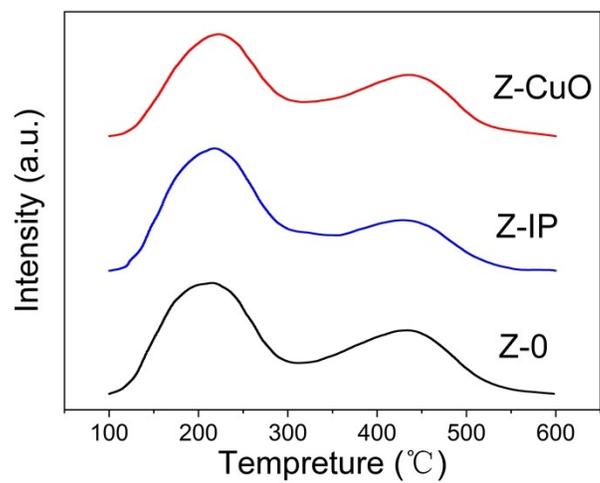


Figure S4. NH₃-TPD profiles of Z-0, Z-CuO and Z-IP

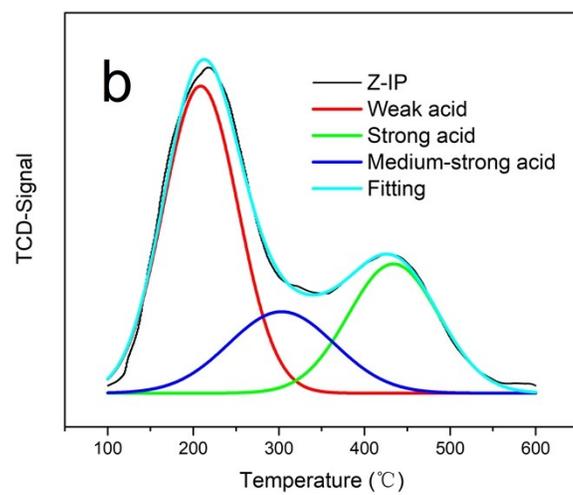
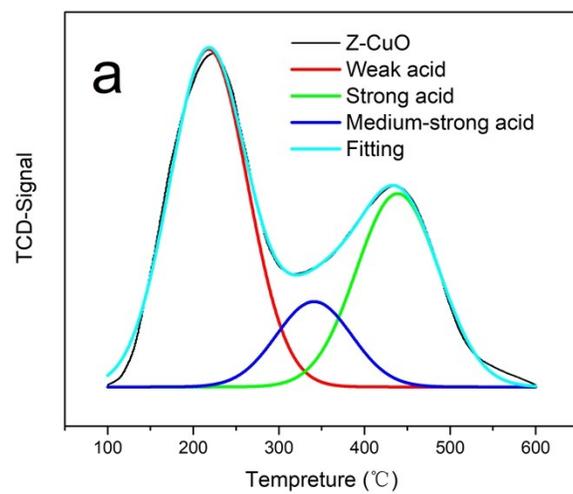


Figure S5. Fitting results of NH_3 -TPD profiles of Z-CuO (a), and Z-IP (b)

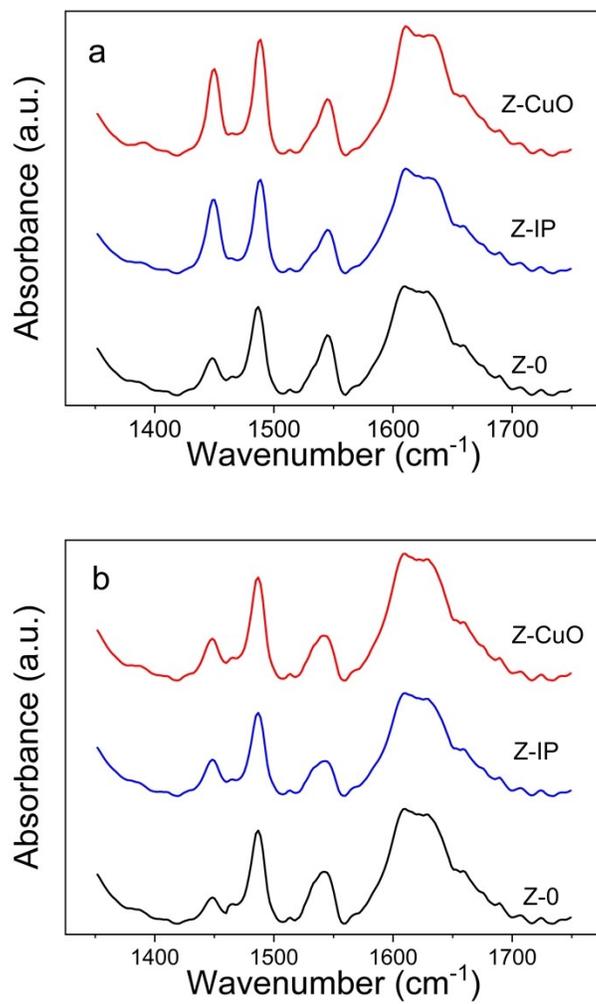


Figure S6. Py-IR profiles of Z-0, Z-CuO, and Z-IP, Desorption at 250°C (a) and 350 °C (b)

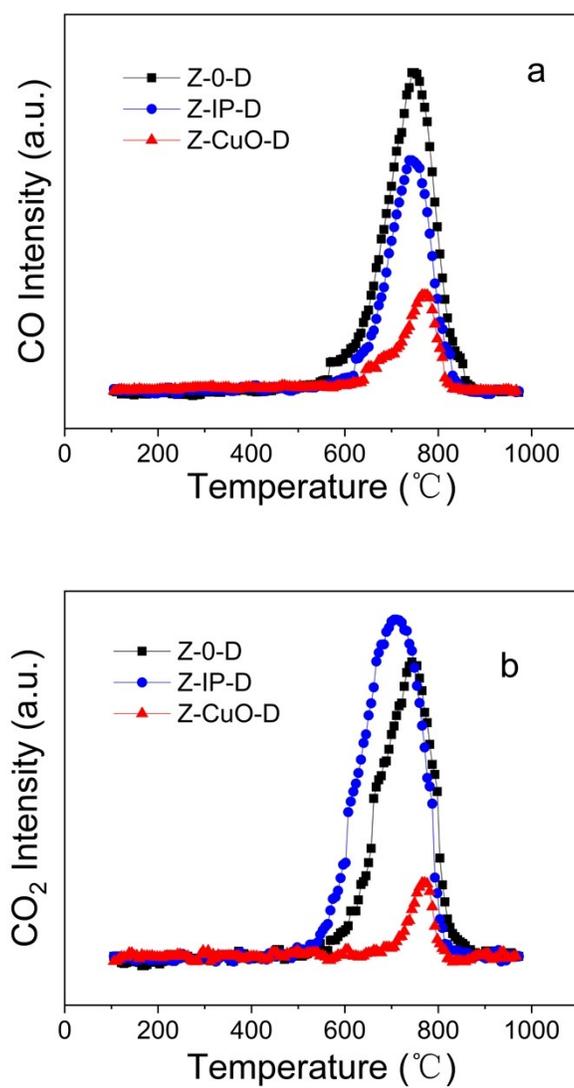


Figure S7. TPO-MS image of deactivated samples, CO peak (a) and CO₂ peak (b)

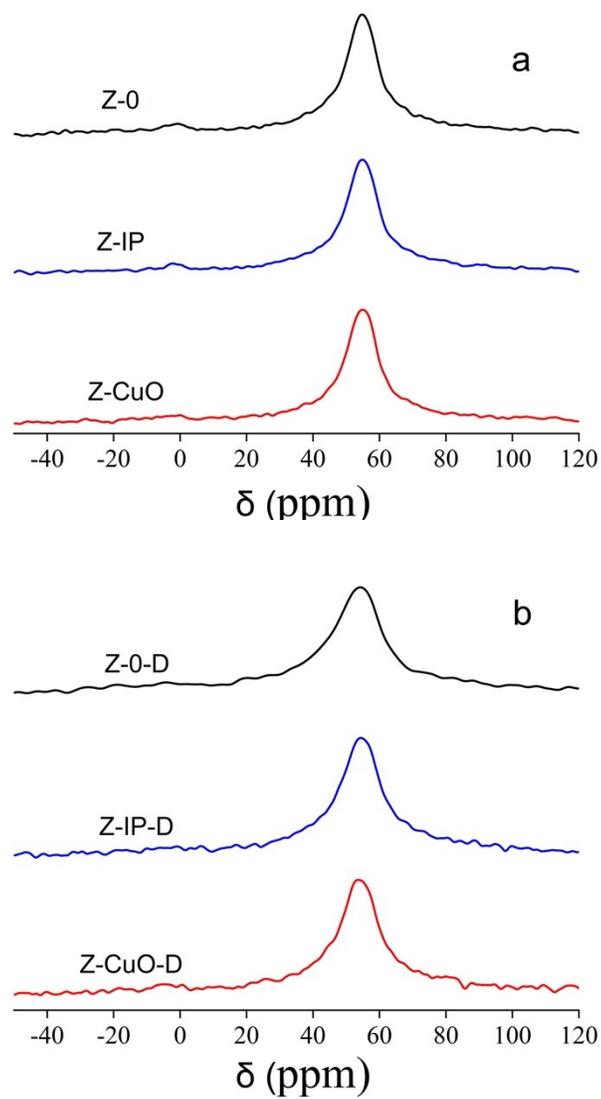


Figure S8. ^{27}Al MAS NMR spectra of the parent and two modified ZSM-5 samples (Z-IP and Z-CuO) before reaction (a) and after reaction (b)

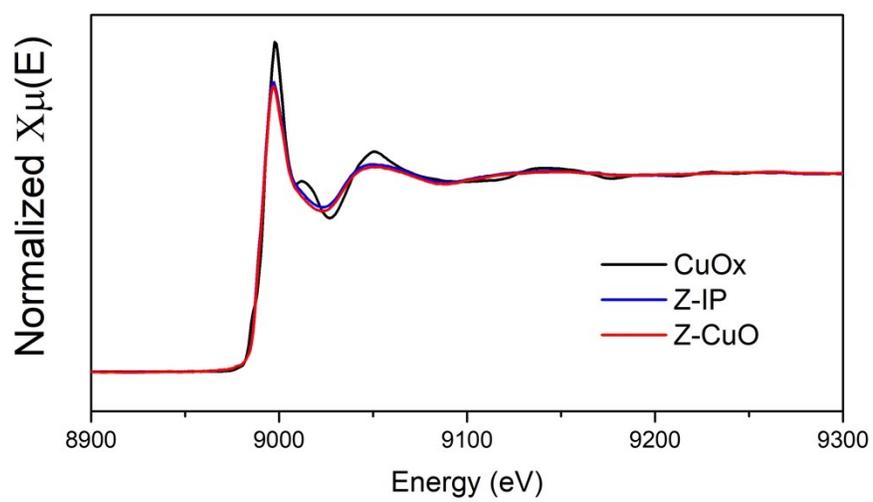


Figure S9. XANES spectra of CuO (black), Z-IP (blue), and Z-CuO (red)

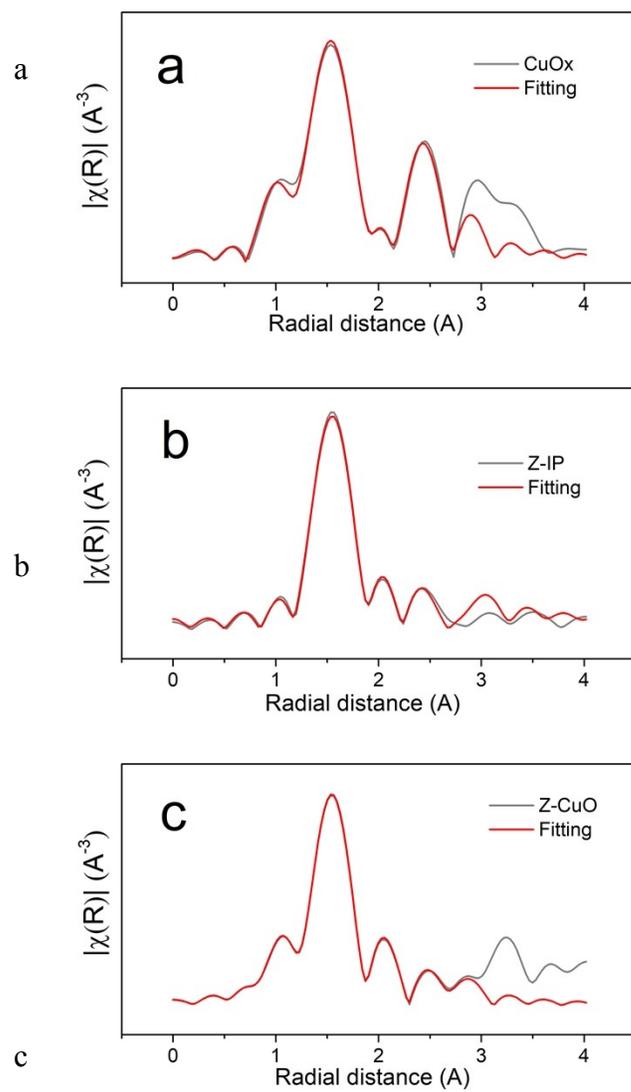


Figure S10. EXAFS fitting spectra of CuO_x (a), Z-IP (b), and Z-CuO (c)

Table S1. Textural properties of Z and Z-IP and Z-CuO samples.

Sample	S_{BET}	S_{micro}	S_{Ext}	V_{mic}	Average Pore Size	Most probable Pore Size	Medium Pore Size
	$(\text{m}^2 \text{g}^{-1})$				(nm)		
Z-0	414	348	65	0.156	2.15	0.67	0.68
Z-IP	411	353	58	0.149	2.25	0.66	0.68
Z-CuO	407	345	62	0.151	2.49	0.69	0.70

Table S2. Acid property of samples obtained by NH₃-TPD measurement

Sample	Peak position (°C)			Acid amount (mmol g ⁻¹)			
	Weak acid	Medium strong acid	Strong acid	Weak acid	Medium Strong acid	Strong acid	Total
Z-0	210.8	313.2	421.3	0.812	0.120	0.545	1.477
Z-IP	208.7	303.3	433.9	0.771	0.289	0.391	1.451
Z-CuO	217.9	341.1	438.8	0.814	0.200	0.496	1.508

Table S3. Amount of carbon deposition on the spent samples calculated by TPO-MS

Sample	Area (a. u.)			Coke amount (Carbon wt%)
	CO	CO ₂	CO+CO ₂	
Z-0-D	60.464	17.789	78.253	5.87
Z-IP-D	40.149	24.073	64.222	4.87
Z-CuO-D	16.180	2.188	18.368	1.11

Table. S4 Acid properties of the parent and samples Z-IP and Z-CuO after steaming treatment

Sample	Peak position (°C)			Retention rate of Acid amount (%)			
	Weak acid	Medium strong acid	Strong acid	Weak acid	Medium Strong acid	Strong acid	Total
Z-0-ST	186.25	253.69	327.82	20.07	25.21	30.10	24.77
Z-IP-ST	190.36	245.47	324.29	20.25	26.43	36.26	28.16
Z-CuO-ST	190.35	269.52	314.346	24.81	34.73	44.03	34.26

Table. S5 Al and Cu concentration of samples before reaction and after regeneration

Sample	Concentration (mg/g)	
	Al	Cu
Z-IP	18.342	3.887
Z-CuO	18.308	3.936
Z-IP-R	15.399	2.137
Z-CuO-R	16.502	3.744

Table. S6 Cu K-edge XANES and EXAFS fit parameters of samples^[a]

Catalysts	Edge energy (eV)	Contribution	N	R(Å)	$\Delta\sigma^2*10^3(\text{Å}^2)$	E0
Z-IP	8989.9	O	2.539	1.957	0.41	-0.190
		O	1.147	2.731	3.30	9.998
		Cu	1.000	2.878	10.40	-2.000
Z-CuO	8989.7	O	3.484	1.952	2.93	-5.120
		O	1.637	2.791	10.50	-1.244
		Cu	1.000	2.897	20.03	-9.998
Z-IP-R	8989.7	O	4.231	1.926	2.99	3.750
		O	1.375	2.706	20.00	9.999
		Cu	9.577	2.997	20.01	9.156
Z-CuO-R	8989.8	O	2.928	1.977	2.98	-1.750
		O	1.725	2.655	20.00	9.997
		Cu	2.182	2.897	20.00	-9.998

[a] N, coordination number; R, distance between absorber and back scatterer atoms.