

Supplementary Materials

Engineering Grain Boundary and Surface Sites of Binary Cu-Mn Catalysts to Boost CO Oxidation

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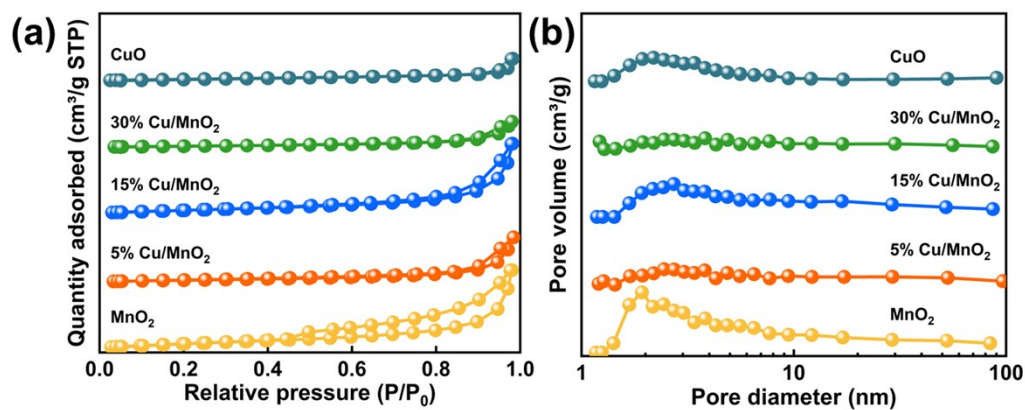


Figure S1. (a) N₂ adsorption-desorption isotherms and (b) pore size distributions of the MnO₂, 5% Cu/MnO₂, 15% Cu/MnO₂, 30% Cu/MnO₂, and CuO catalysts.

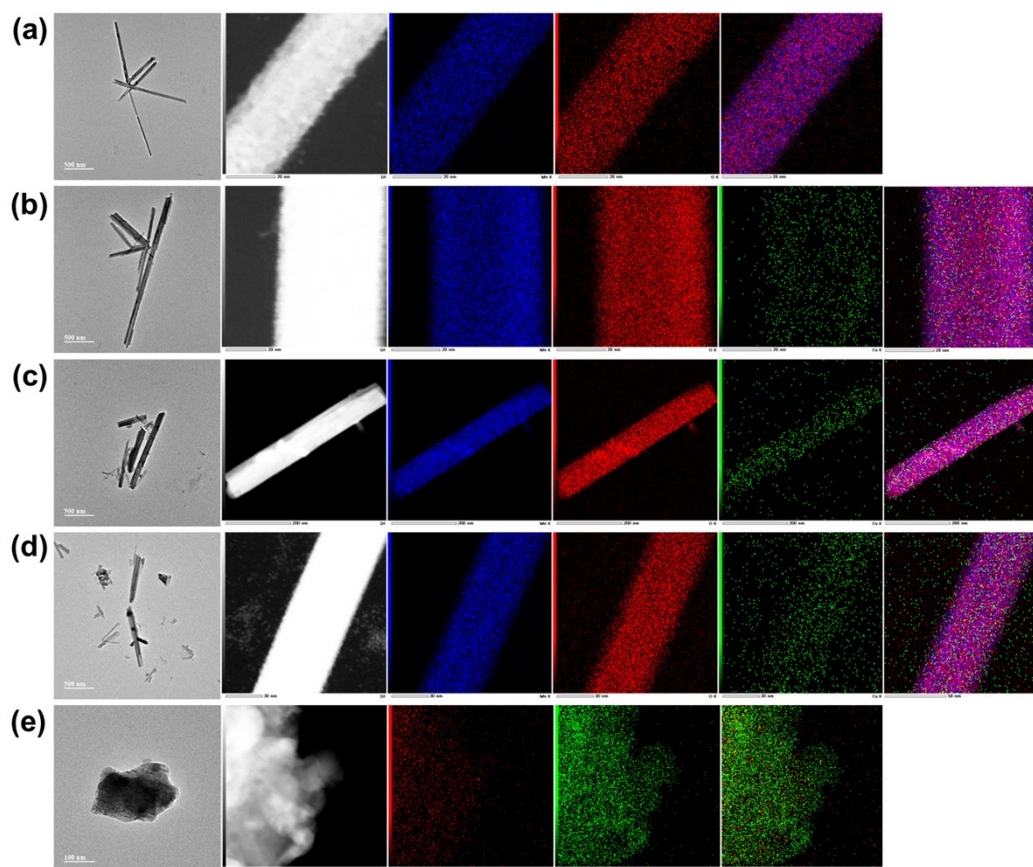


Figure S2. Typical HRTEM, HAADF-STEM, and EDS mapping images of (a) MnO₂, (b) 5% Cu/MnO₂, (c) 15% Cu/MnO₂, (d) 30% Cu/MnO₂, and (e) CuO catalysts.

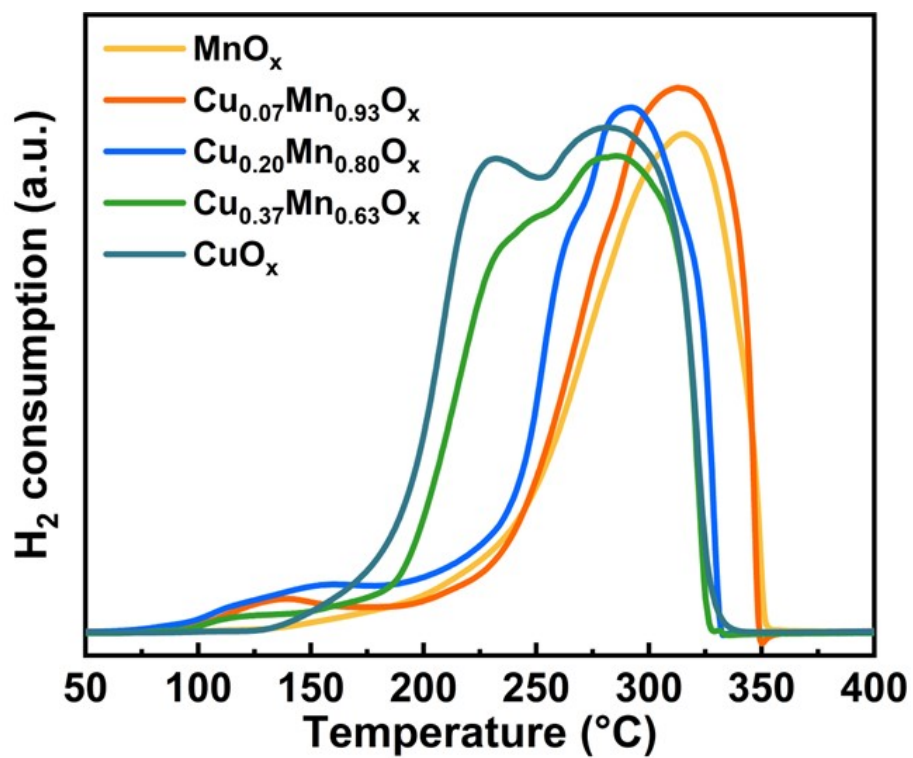


Figure S3. H_2 -TPR curves of the MnO_2 , 5% Cu/MnO_2 , 15% Cu/MnO_2 , 30% Cu/MnO_2 , and CuO catalysts.

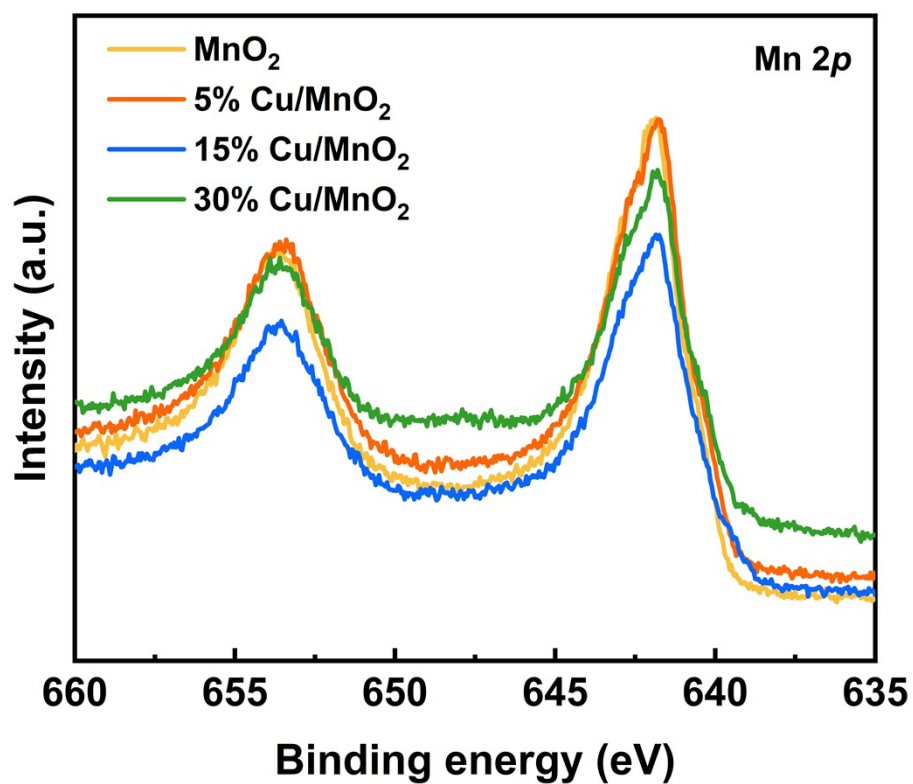


Figure S4. Mn 2p XPS spectra of the MnO₂, 5% Cu/MnO₂, 15% Cu/MnO₂, and 30% Cu/MnO₂ catalysts.

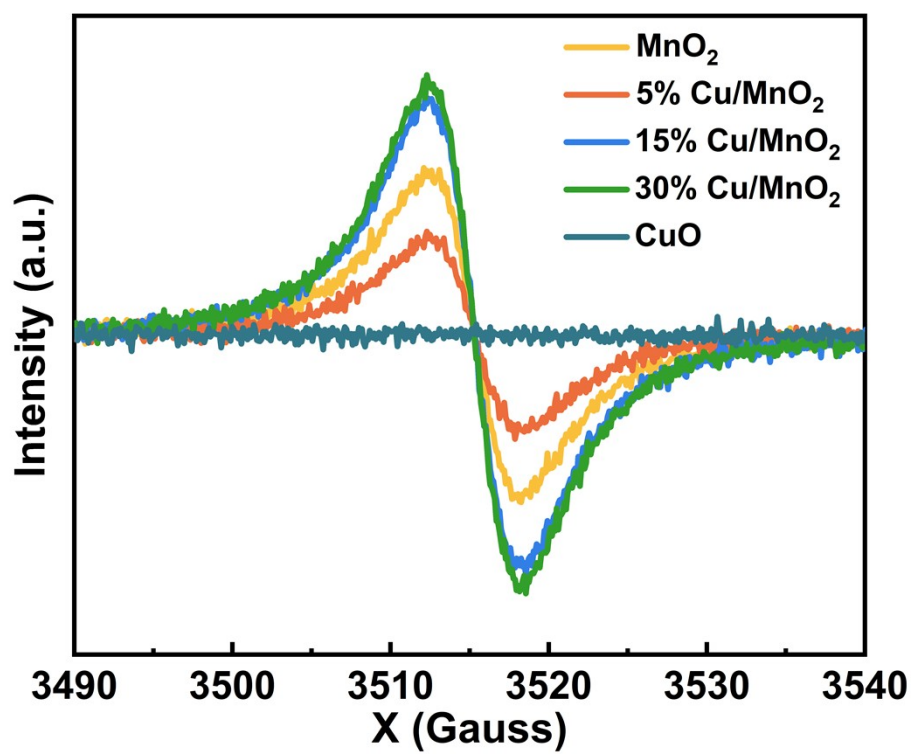


Figure S5. EPR profiles of the MnO₂, 5% Cu/MnO₂, 15% Cu/MnO₂, 30% Cu/MnO₂, and CuO catalysts.

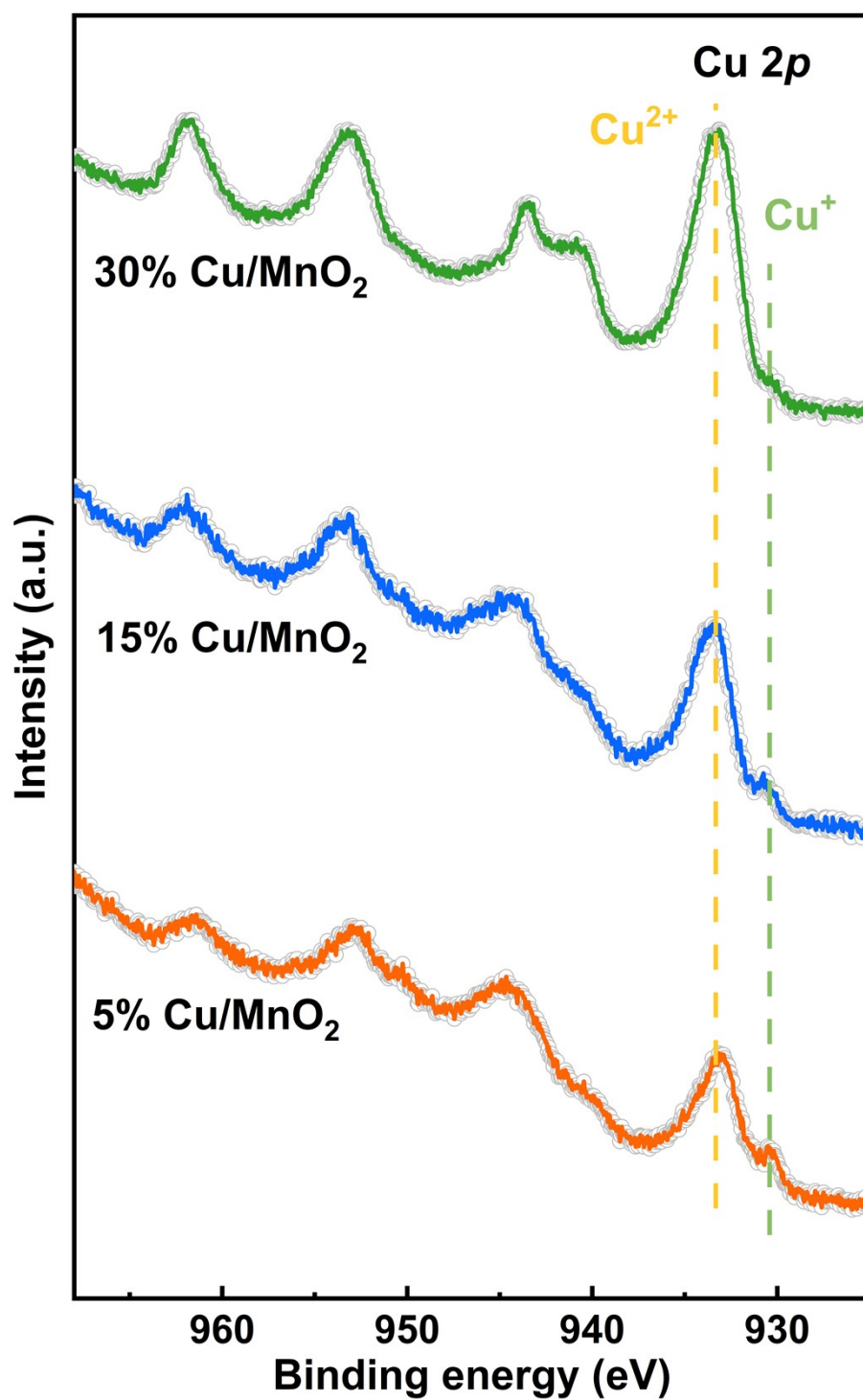


Figure S6. Cu 2p XPS spectra of the 5% Cu/MnO₂, 15% Cu/MnO₂, and 30% Cu/MnO₂ catalysts.

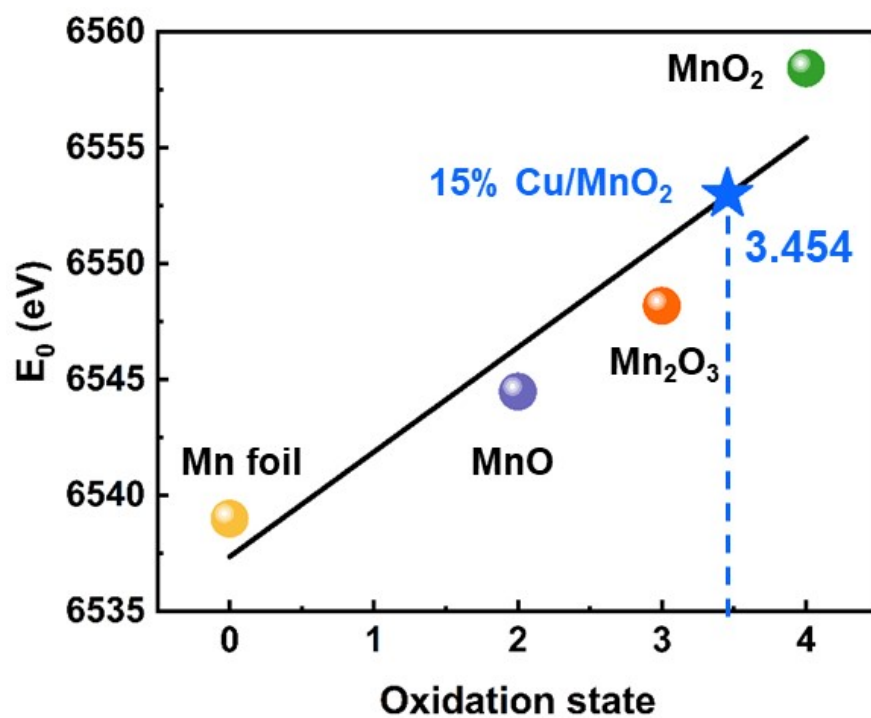


Figure S7. Linear combination analysis for the position of absorption edges in XANES curve of the Mn *K*-edge for the 15% Cu/MnO₂ catalyst.

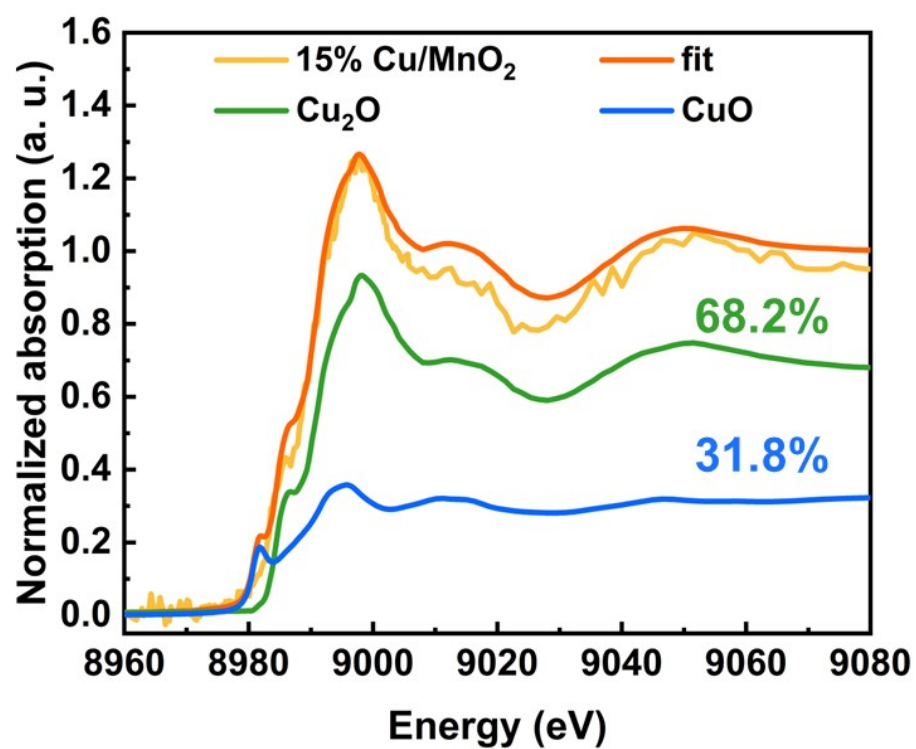


Figure S8. Linear combination analysis for the XANES curve of the Cu *K*-edge for the 15% Cu/MnO₂ catalyst.

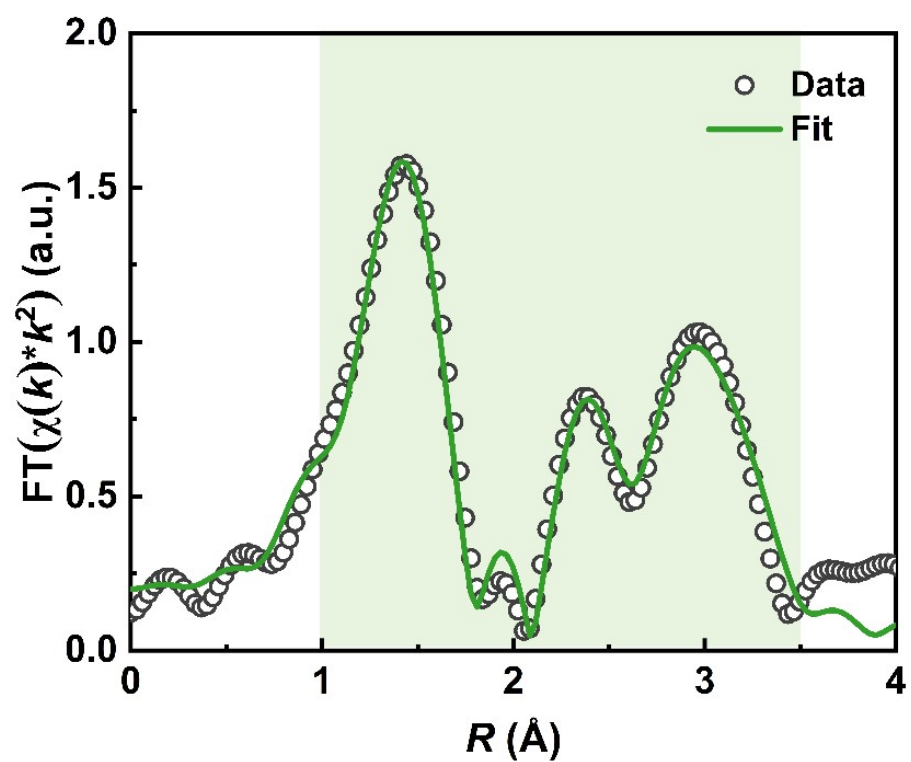


Figure S9. Fourier transforms of the experimental and fitted EXAFS spectra in R -space of the standard MnO_2 at the Mn K -edge.

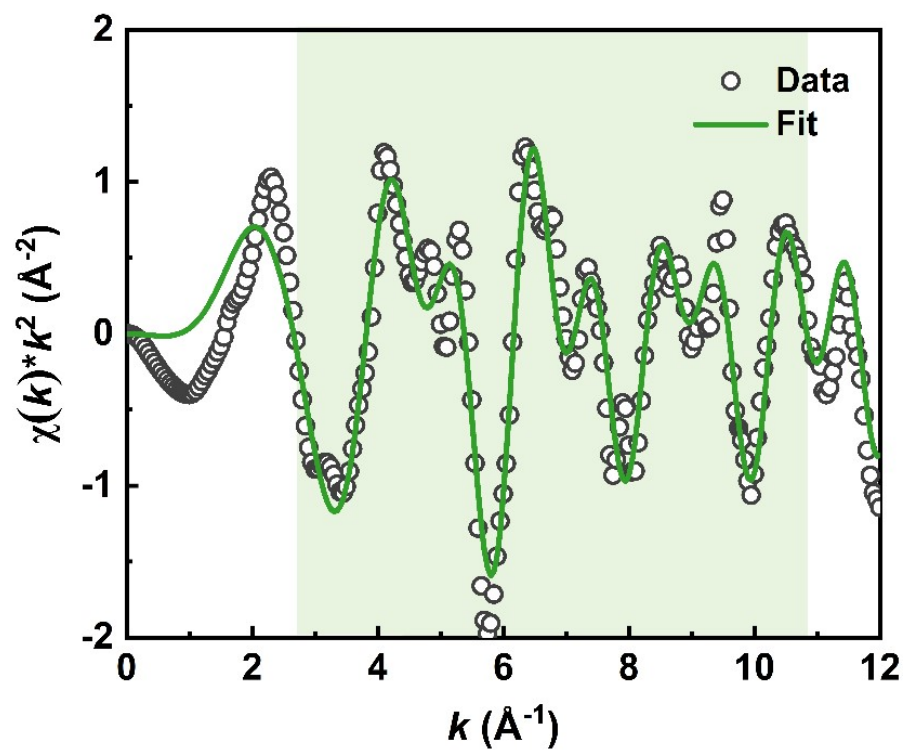


Figure S10. Fourier transforms of the experimental and fitted EXAFS spectra in k -space of the standard MnO_2 at the Mn K -edge.

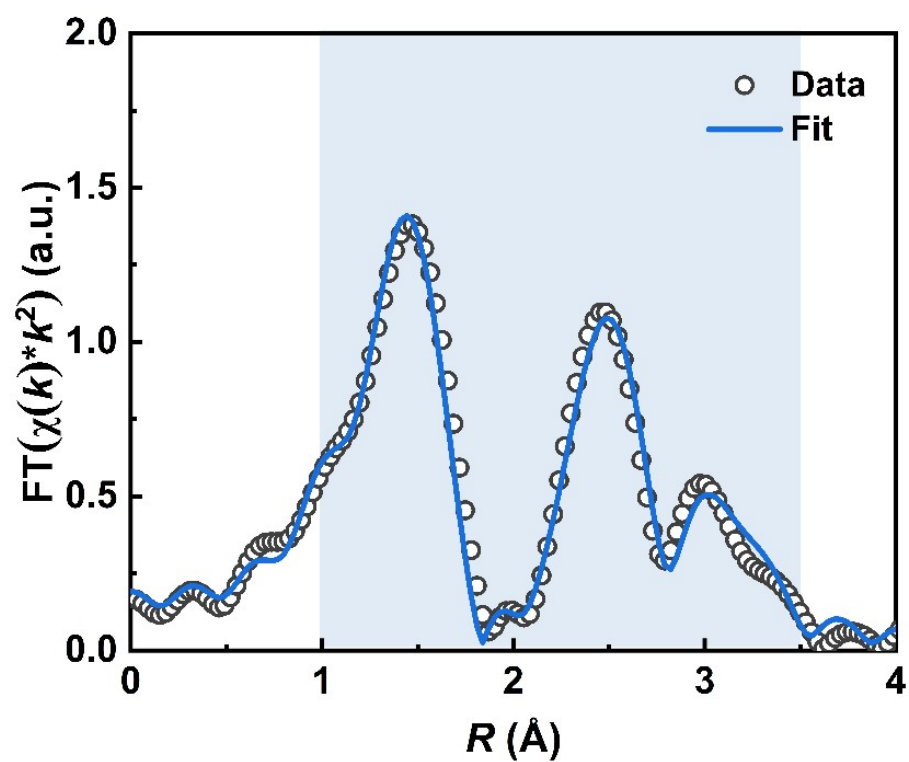


Figure S11. Fourier transforms of the experimental and fitted EXAFS spectra in R -space of the 15% Cu/MnO₂ catalyst at the Mn K -edge.

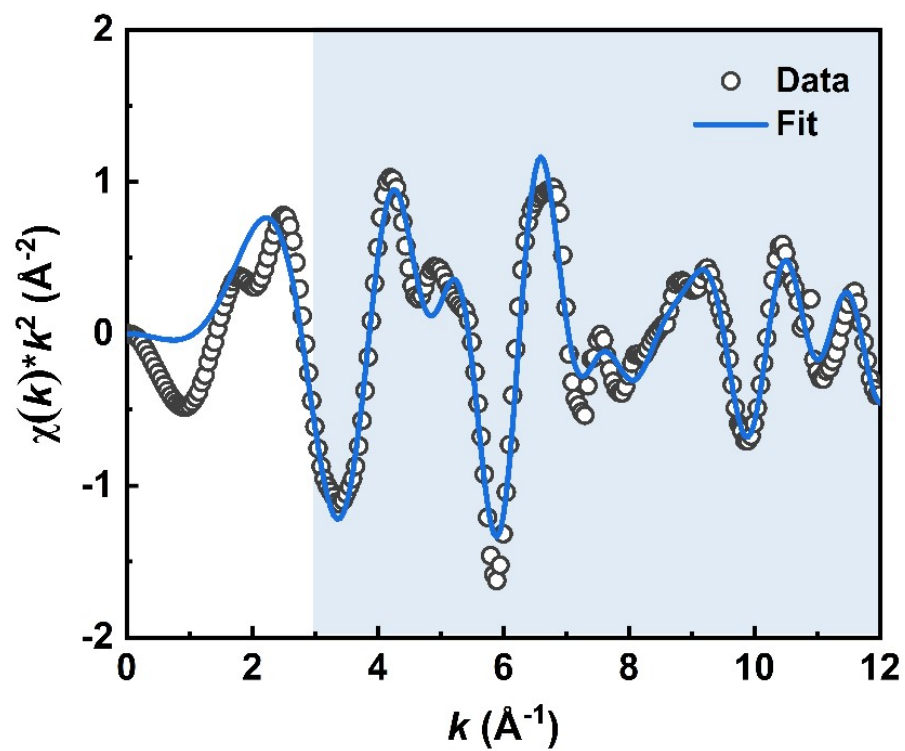


Figure S12. Fourier transforms of the experimental and fitted EXAFS spectra in k -space of the 15% Cu/MnO₂ catalyst at the Mn K -edge.

Table S1. Structural parameters of Mn foil, the standard MnO₂, and the 15% Cu/MnO₂ catalyst from the EXAFS fitting.

Sample	Shell	CN ^a	R (Å) ^b	σ ² (Å ²) ^c	ΔE ₀ ^d	R factor ^e
Mn foil	Mn-Mn	2	2.47±0.02	0.006±0.002	4.4±2.5	0.015
	Mn-O	4.6±0.7	1.89±0.01	0.001±0.002		
MnO ₂	Mn-Mn ₁	3.6±3.5	2.86±0.04	0.009±0.009	-4.0±2.1	0.011
	Mn-Mn ₂	4.2±2.0	3.43±0.02	0.001±0.003		
15% Cu/MnO ₂	Mn-O	4.6±0.5	1.89±0.01	0.003±0.001		
	Mn-Mn ₁	4.5±1.5	2.86±0.01	0.006±0.003	-1.1±1.2	0.014
	Mn-Mn ₂	1.8±1.2	3.43±0.01	0.001±0.004		

^aCN: coordination numbers. ^bR: bond distance. ^cσ²: Debye-Waller factors.

^dΔE₀: the inner potential correction. ^eR factor: goodness of fit. S₀² was set to 0.61 for Mn samples, according to the experimental EXAFS fit of Mn foils reference by fixing CN as the known crystallographic value.