

Supporting Information

Designing bimetallic IrRu nanoparticles on oxygen-deficient WO₃ for efficient NO reduction by CO

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Table S1 The BET specific surface area, pore volume, and pore size of WO₃ support,

Ir/WO₃, Ru/WO₃ and IrRu/WO₃ catalysts

Sample	BET specific surface area (m ² /g)	Pore size (nm)	Pore Volume (cm ³ /g)
WO ₃	2.6	31.15	0.0405
Ir/WO ₃	7.18	9.99	0.0359
Ru/WO ₃	1.98	50.82	0.0503
IrRu/WO ₃	6.58	11.16	0.0367

Table S2 CO-SCR performance over the various referenced samples

Catalyst	Metal loading	Ir:Ru	Feed composition	Contact time (mL/h·g cat)	Optimum CO-SCR performance			Ref.	
					Temp.	NO _x conv.	CO conv.		N ₂ sel.
IrRu/WO ₃	5 wt%	1:1	500 ppm NO, 5000 ppm CO, 1.5% O ₂ , and 3% H ₂ O	15000	350 °C	87%	100%	92%	This work
IrRu/Al ₂ O ₃	5 wt%	1:3	50 ppm NO, 7000 ppm CO, 5 % O ₂ , 5 % H ₂ O, and 5% CO ₂	120000	225 °C	75%	100%	94%	41
IrRu/Al ₂ O ₃	2.32 wt%	1:2.7	50 ppm NO, 0.7 % CO, 5% O ₂ , and 10 % H ₂ O	100000	200 °C	82%	98%	88%	20
IrRu/ZSM-5	0.76 wt%	1:1	50 ppm NO, 3000 ppm CO, and 5 % O ₂	100000	250 °C	90%	100%	-	19
IrRu/Al ₂ O ₃	3.05 wt%	1:1	200 ppm NO, 7000 ppm CO, 5 % O ₂ , and 10 % H ₂ O	100000	175 °C	70%	100%	70%	23
IrRu/TiO ₂	3.05 wt%	1:1	200 ppm NO, 7000 ppm CO, 5 % O ₂ , and 10 % H ₂ O	100000	200 °C	34%	98%	50%	23
IrRu/Al ₂ O ₃	3.05 wt%	1:1	50 ppm NO, 7000 ppm CO, 5% O ₂ and 10 % H ₂ O	100000	175 °C	91%	100%	78%	22
IrRu/Al ₂ O ₃	5 wt%	1:3	50 ppm NO, 7000 ppm CO, and 5 % O ₂	120000	200 °C	88%	90%	86%	21

Table S3 Atomic concentration on catalyst surface in XPS results.

Catalyst	Surface atomic ratio (%)					
	Ir ⁰ /Ir _{total}	Ir ⁴⁺ /Ir _{total}	Ru ⁰ /Ru _{total}	Ru ⁴⁺ /Ru _{total}	O _α /O _{total}	O _β /O _{total}
Ir/WO ₃	0.46	0.54	-	-	0.15	0.44
Ru/WO ₃	-	-	0.70	0.30	0.50	0.32
IrRu/WO ₃	0.64	0.36	0.77	0.23	0.21	0.45

Table S4 Adsorption energy of adsorbate gases on catalyst models

Adsorbate gas	Adsorption energy (eV)		
	Ir(111)	Ir ₃ Ru ₁ (111)	Ir ₃ Ru ₁ (111)-O _v
NO	-1.58	-3.129	-
CO	-2.395	-2.816	-
O ₂	-1.838	-1.795	-1.691

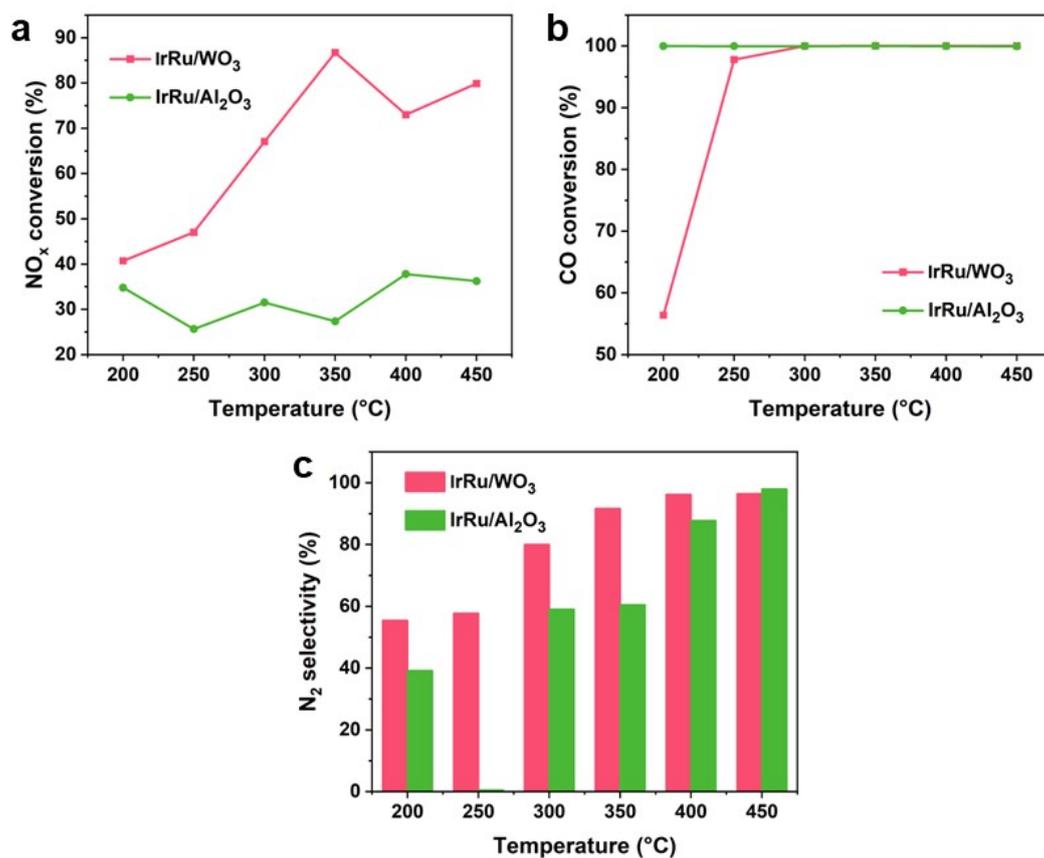


Fig. S1 (a) NO_x conversion, (b) CO conversion, (c) N₂ selectivity over reduced IrRu/WO₃ and IrRu/Al₂O₃ catalysts. Feed composition (standard feed): 500 ppm NO, 5000 ppm CO, 1.5% O₂, and 3% H₂O balanced with Ar (Contact time 15000 mL/h•g catalyst). Pretreatment conditions involved a 10% H₂ flow balanced with Ar, reduced at 500 °C for 1 h.

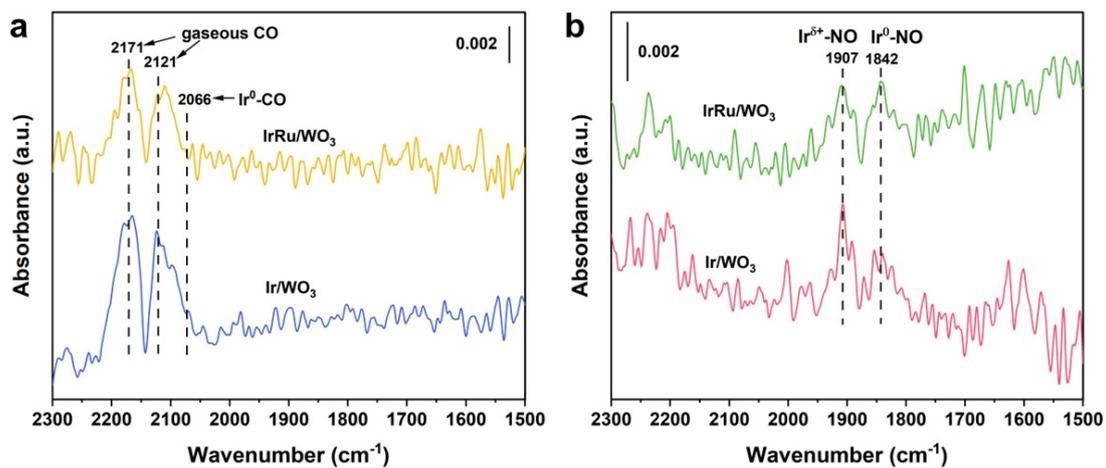


Fig. S2 FT-IR spectra of the reduced catalysts after exposure to (a) CO and (b) NO feed stream (5000 ppm CO/3000 ppm NO, balanced with Ar) for 30 min at 35 °C (the samples were undiluted).

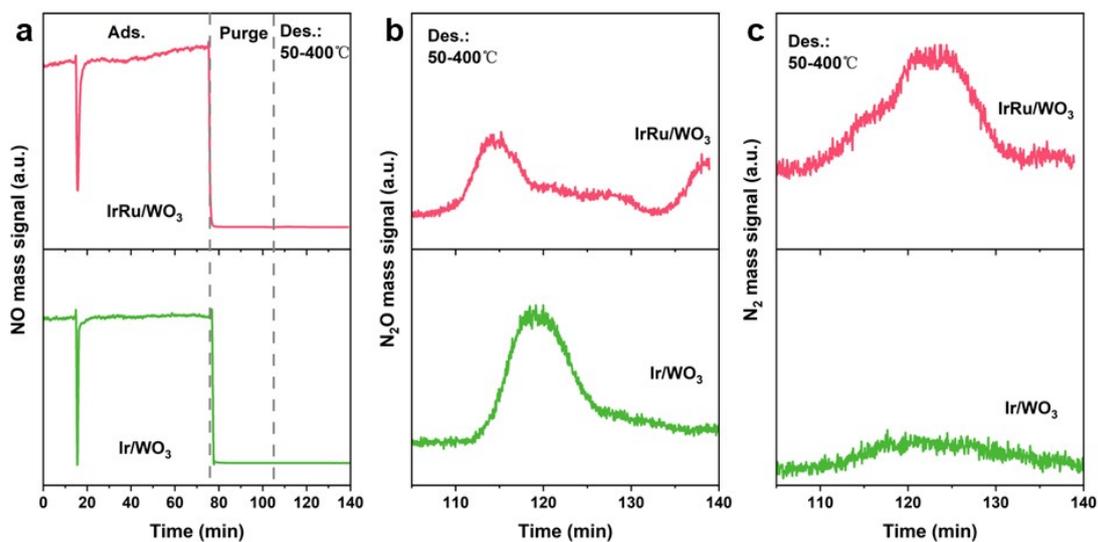


Fig. S3 The MS signals of (a) NO, (b) N₂O and (c) N₂ during the NO-TPD experiments of the catalysts. Adsorption step: 5000 ppm NO/Ar, 50 °C. Purging step: Ar, 50 °C. Desorption step: Ar, 50~400 °C, ramping at 10 °C/min.

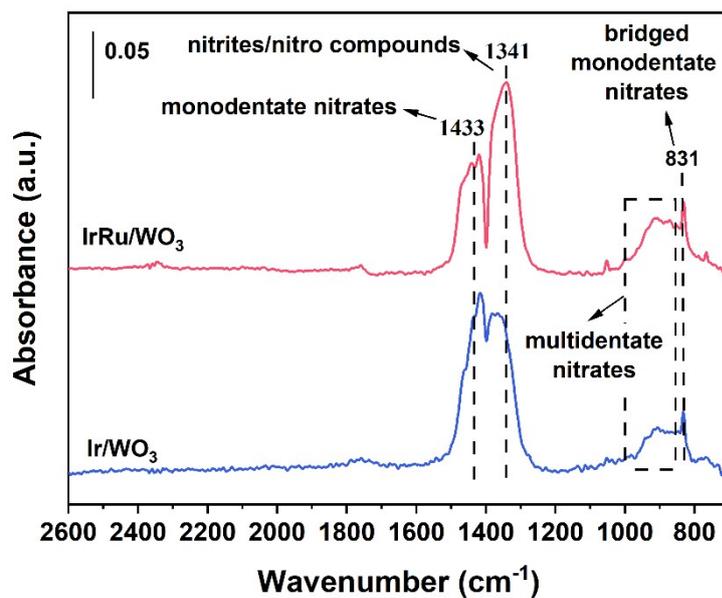


Fig. S4 FT-IR spectra of the reduced catalysts after exposure to NO-CO-O₂ feed stream (0.3% NO, 3% CO, 5% O₂) for 30 min, followed by Ar purging for 1 h 30 min at 350 °C (the samples were diluted with KBr).

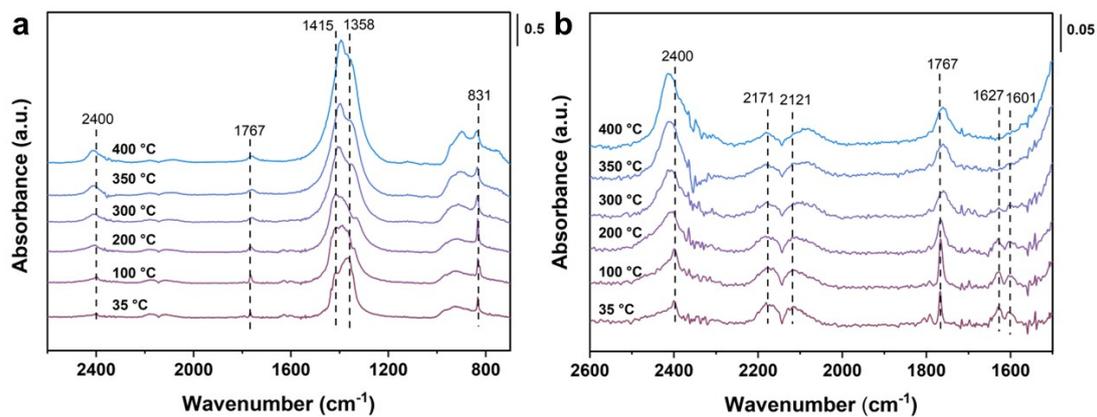


Fig. S5 Temperature-dependent *in-situ* DRIFTS spectra during adsorption of NO + CO + O₂ (0.3% NO, 3% CO, 5% O₂) for IrRu/WO₃ catalyst. The spectra are presented in two ranges: (a) from 2600 to 700 cm⁻¹ and (b) from 2600 to 1500 cm⁻¹, with the samples being diluted with KBr.

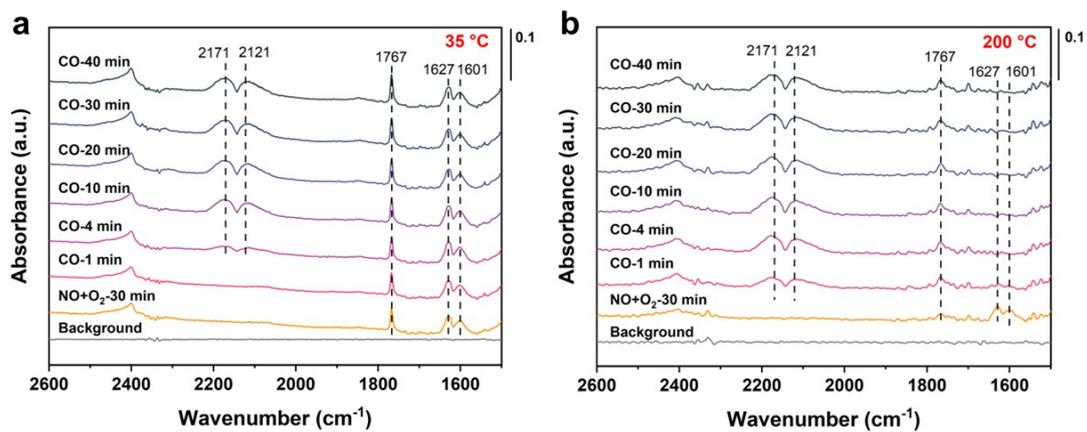


Fig. S6 *In-situ* DRIFTS spectra for the adsorption of CO after pre-adsorption of NO + O₂ at (a) 35 °C and (b) 200 °C for IrRu/WO₃ (the samples were diluted with KBr).

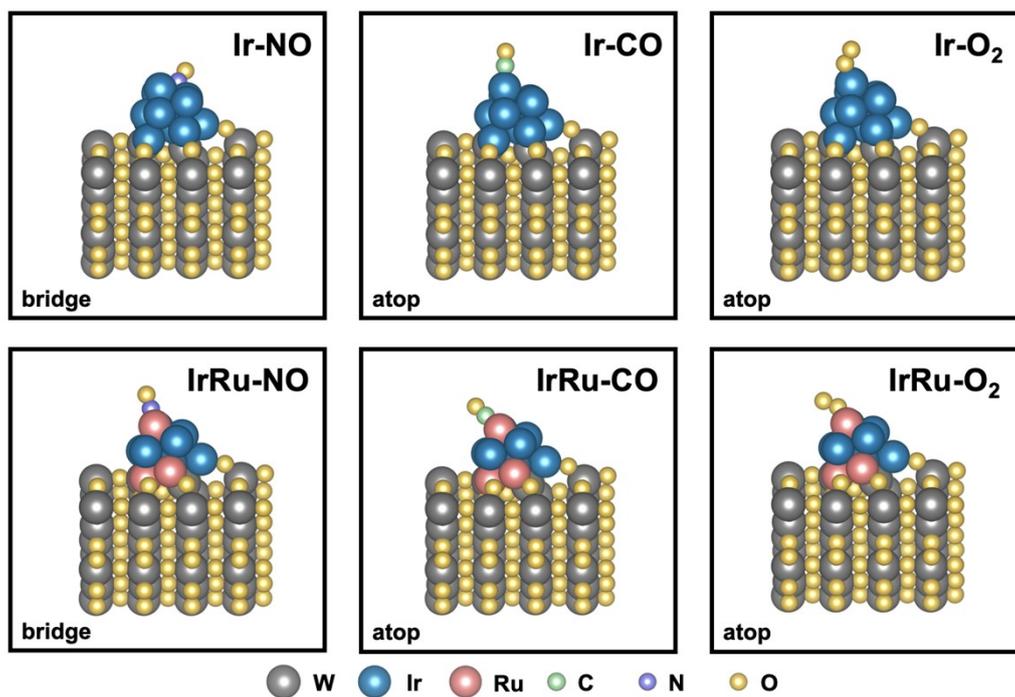


Fig. S7 Optimized Ir(111) and Ir₃Ru₁(111) slab models with different adsorbates. The most stable site for each adsorbate is mentioned under each figure.

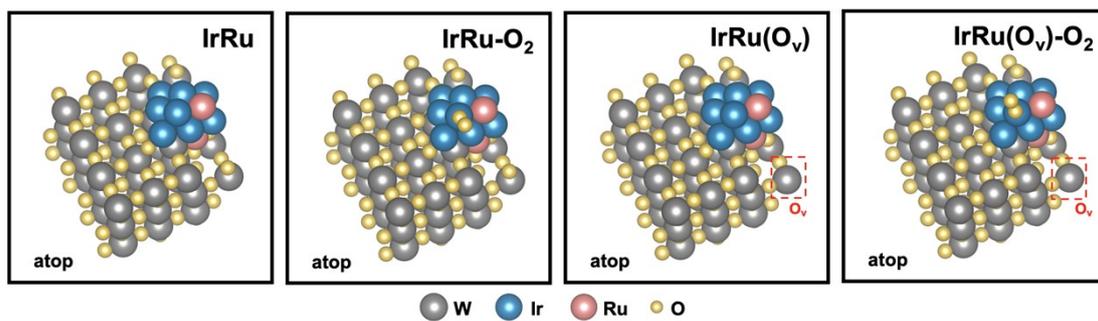


Fig. S8 Optimized $\text{Ir}_3\text{Ru}_1/\text{WO}_{2.92}$, $\text{Ir}_3\text{Ru}_1/\text{WO}_{2.92}(\text{O}_v)$ models and their models with O_2 adsorbate gas.