

Supporting information

Selective catalytic reduction of NO_x with NH₃ on the short-range ordered W-O-Fe structure with high thermal stability

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Including:

Figure S1-S4

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Figures

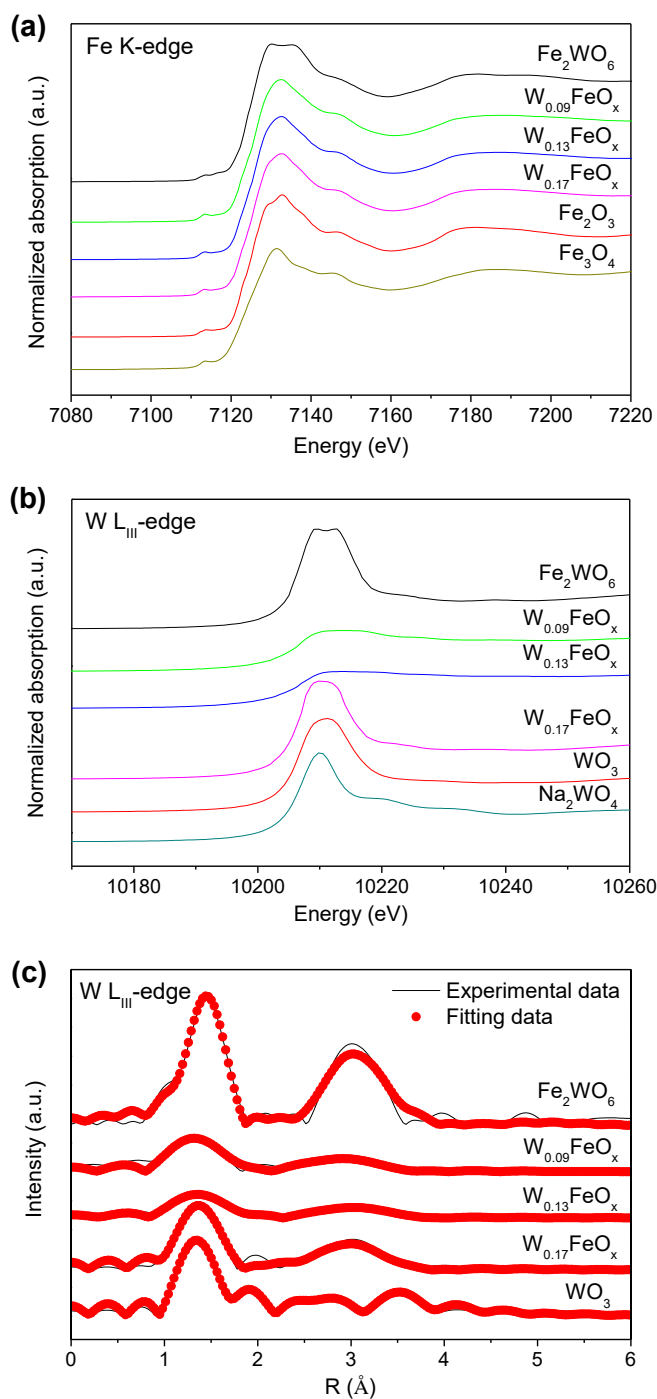


Figure S1. (a) Normalized Fe K-edge XANES spectra, (b) normalized W L_{III} -edge XANES spectra, and (c) quantitative curve fitting in RSF curves for W_dFeO_x catalysts and the reference samples.

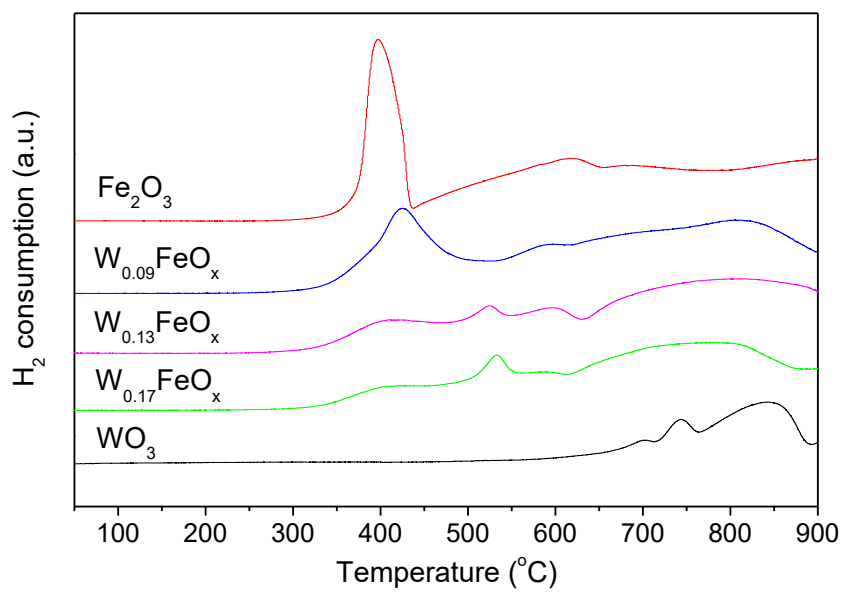


Figure S2. H₂-TPR profiles for Fe₂O₃, WO₃, and W_dFeO_x catalysts.

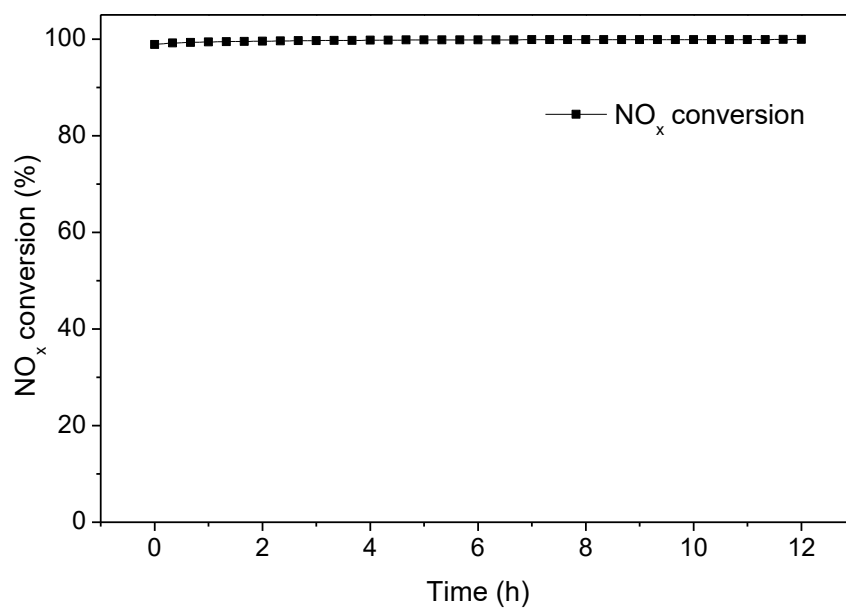


Figure S3. NO_x conversion of W_{0.13}FeO_x-800 versus reaction time in the SCR reaction feed at 300 °C.

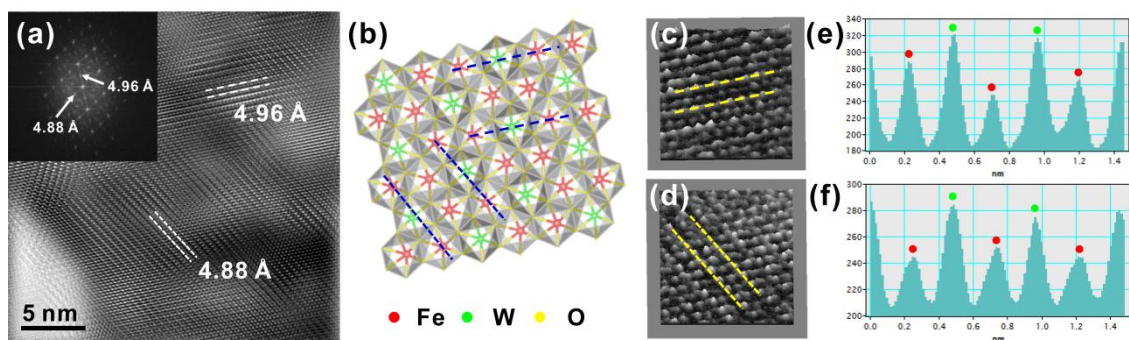


Figure S4. (a) HRTEM image with the corresponding FT image of Fe_2WO_6 ; (b) simulated model of Fe_2WO_6 viewed along the $[1\ 0\ 0]$ direction; (c, d) computed 3D images; and (e, f) the corresponding profile line analysis of the periodic ordered W-O-Fe structure.

Tables

Table S1. Structural parameters of WO_3 , W_aFeO_x , and Fe_2WO_6 obtained from W L_{III} -edge EXAFS analysis.

Sample	Shell	N	R (Å)	σ^2 (Å ²)	ΔE_0 (eV)	R-factor
WO_3	W-O	5.0	1.770202	0.001142	3.7	0.000036581
	W-O	2.0	2.624901	0.001173	-19.0	
	W-W	2.0	3.747567	0.012522	24.2	
$\text{W}_{0.09}\text{FeO}_x$	W-O	5.7	1.790402	0.001927	5.0	0.032052842
	W-Fe	1.5	3.181191	0.025760	21.9	
$\text{W}_{0.13}\text{FeO}_x$	W-O	5.8	1.801378	0.001355	8.6	0.026921577
	W-Fe	1.6	3.372399	0.027803	16.4	
$\text{W}_{0.17}\text{FeO}_x$	W-O	5.7	1.811347	0.004777	4.1	0.033862166
	W-Fe	1.6	3.226850	0.023830	22.7	
Fe_2WO_6	W-O	6.0	1.875802	0.006897	6.9	0.001014360
	W-Fe	2.0	3.250363	0.015747	29.1	

Table S2. XPS data for W_aFeO_x catalysts.

Sample	W mass concentration %	Fe mass concentration %	W/Fe molar ratio
WO_3	78.18	--	--
$W_{0.09}FeO_x$	23.52	47.06	0.40
$W_{0.13}FeO_x$	23.47	51.45	0.29
$W_{0.17}FeO_x$	30.91	45.68	0.24
Fe_2O_3	--	52.26	--