Electronic Supplementary Information (ESI)

Tuning Electronic States of Catalytic Sites Enhances SCR Reactivity of Hexagonal WO_3 by Mo Framework Substitution†

Yaxin Chen,[a,§] Zichenxi Dong,[a,§] Zhiwei Huang,[a] Meijuan Zhou,[a] Jiayi Gao,[a] Junxiao Chen,[a] Chao Li,[a] Zhen Ma,[a] Jianmin Chen,[a] and Xingfu Tang*[,a,b]

[a] Institute of Atmospheric Sciences, Shanghai Key Laboratory of Atmospheric Particle Pollution & Prevention (LAP^3), Department of Environmental Science & Engineering, Fudan University, Shanghai 200433, China

[b] Jiangsu Collaborative Innovation Center of Atmospheric Environment and Equipment Technology (CICAEET), Nanjing University of Information Science & Technology, Nanjing, 210044, China

[§] These authors contributed equally to this work.

[*] Corresponding author: Phone: +86-21-65642997; fax: +86-21-65643597; e-mail: tangxf@fudan.edu.cn.

Pages S1-S11

Tables S1-S3

Figures S1-S9

Contents

Table S1. Structure parameters of K/Mo-HWO, Mo-HWO, and HWO determined by the Rietveld refinement of the corresponding SXRD data.

Samples	Atom	*x*	*y*	*z*	Occupancy
K/Mo-HWO	K	0	0	0	0.28
	W/Mo	0.5	0	0	1.0
	O1	0.5	0	0.5	1.0
	O2	0.21	0.42	0	1.0

Table S2. Crystallographic data and details of HWO, Mo-HWO, and K/Mo-HWO in the SXRD data collections and the Rietveld refinements.

Parameters	Crystallographic data
Sample	K/Mo-HWO
Crystal system	hexagonal
Space group	*P*6/*mmm*
a (Å)	7.318
c (Å)	3.807
V (Å^3)	176.6
R_p [a] (%)	3.28
R_{wp} [b] (%)	5.19
R_{exp} [c] (%)	1.74
χ^2 [d]	8.89
Wavelength (Å)	0.6883
2θ range (°)	5-35
2θ step width (°)	0.02

[a] R_p, the unweighted profile factor;

[b] R_{wp}, the weighted profile factor;

[c] R_{exp}, the expected R parameter;

[d] χ^2, the goodness of fitting, defined as the square of the ratio of R_{wp}/R_{exp}.

Table S3. Detailed data of XPS of W and Mo and their calculated average oxidation states in HWO and Mo-HWO as determined by W 4*f* and Mo 3*p* XPS analyses.

Sample	W^{6+} (eV/%)	W^{5+} (eV/%)	W^{4+} (eV/%)	Average oxidation state of W	Mo^{6+} (eV/%)	Mo^{5+} (eV/%)	Average oxidation state of Mo
HWO	35.3/83	34.4/17	–	5.8	–	–	–
Mo-HWO	35.3/53	34.4/40	32.3/7	5.5	232.5/80	231.5/20	5.8

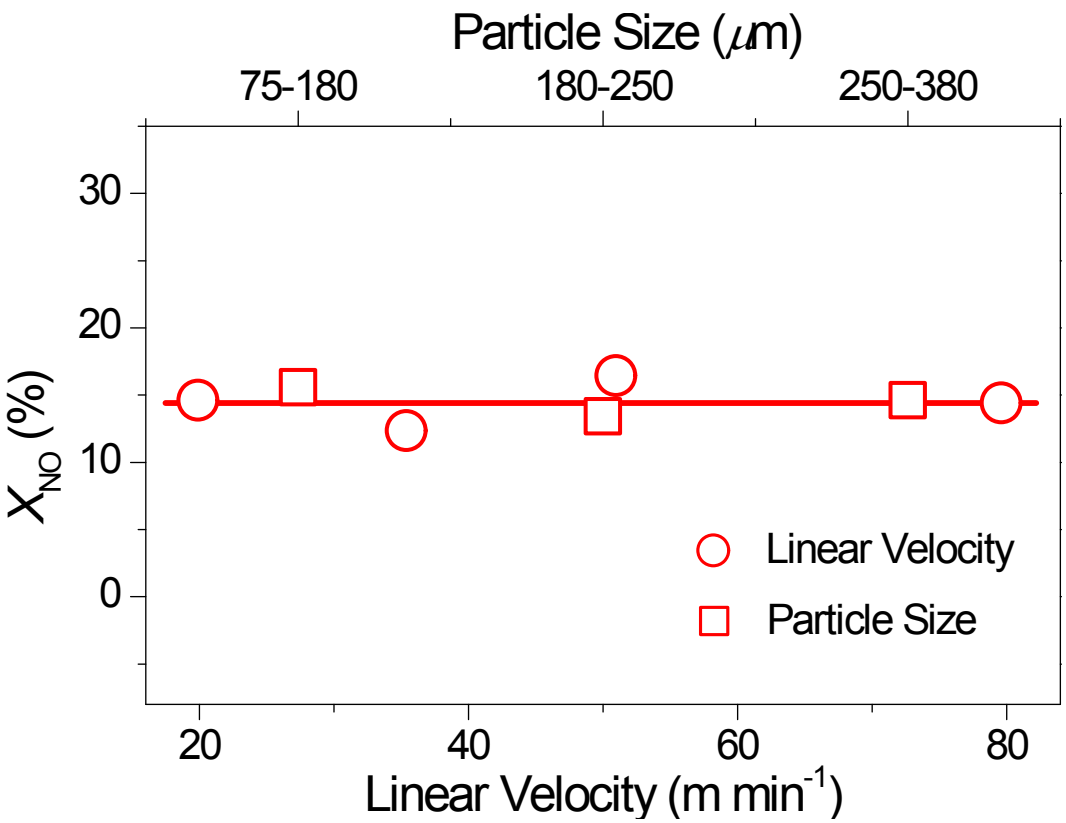

Fig. S1. NO conversions (X_{NO}) on Mo-HWO as a function of the linear velocity of the feed gas (red circle) and the particle size (red square). Conditions: temperature = 300 °C, NO = NH_3 = 500 ppm, O_2 = 3.0 vol%, and balance N_2, gas flow rate = 1000 mL min^{-1}.

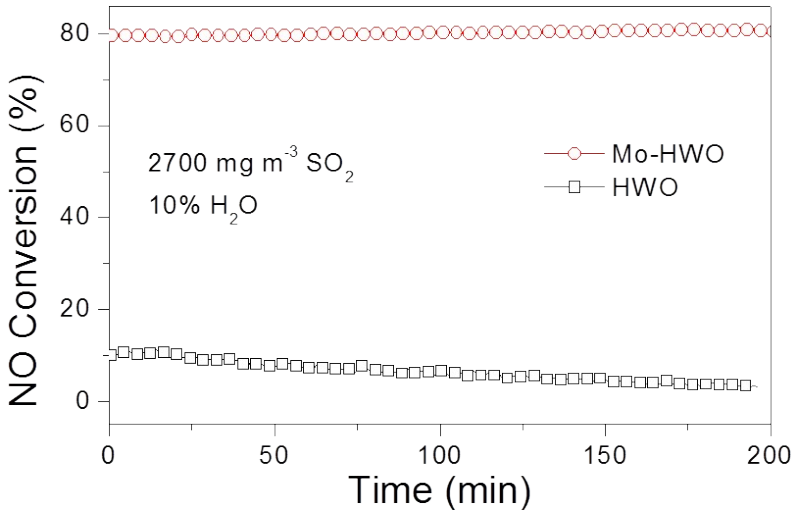

Fig. S2. NO conversions with time on stream over Mo-HWO and HWO at 350 °C. Reaction conditions: 1000 ppm NH_3, 1000 ppm NO, 3 vol.% O_2, 2700 mg m^{-3} SO_2, 10 vol.% H_2O, balanced by N_2, and the gas hourly space velocity (GHSV) 32,000 h^{-1}.

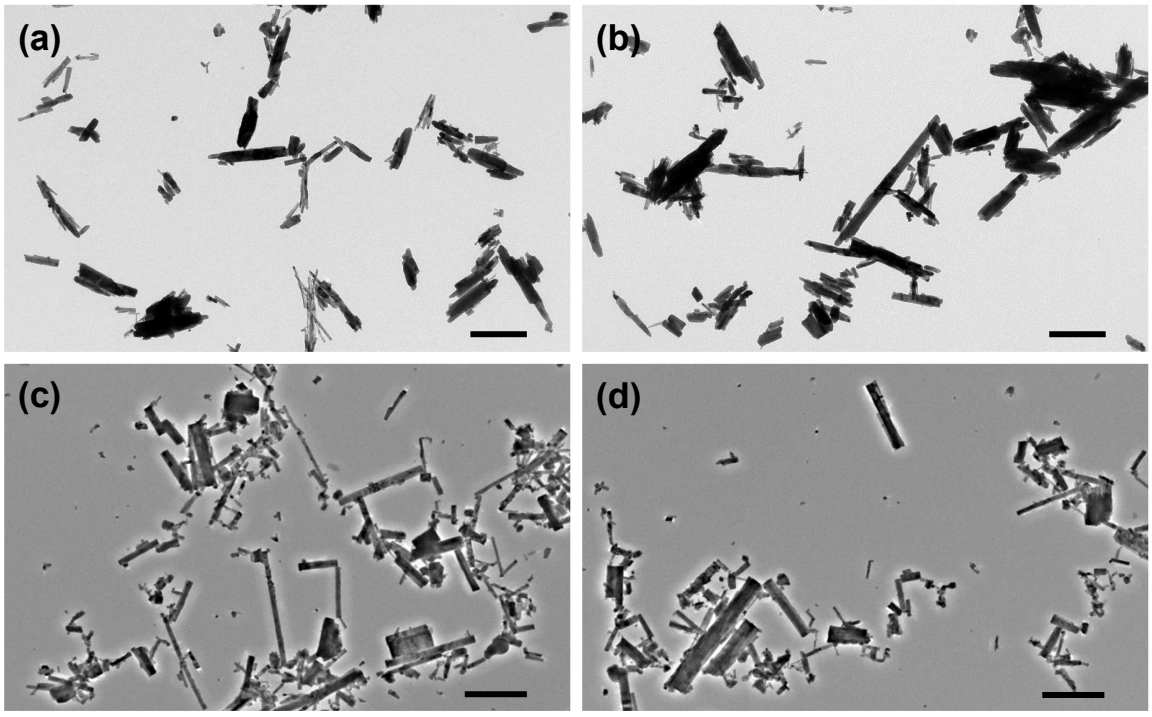

Fig. S3 TEM images of HWO (a,b) and Mo-HWO (c,d).

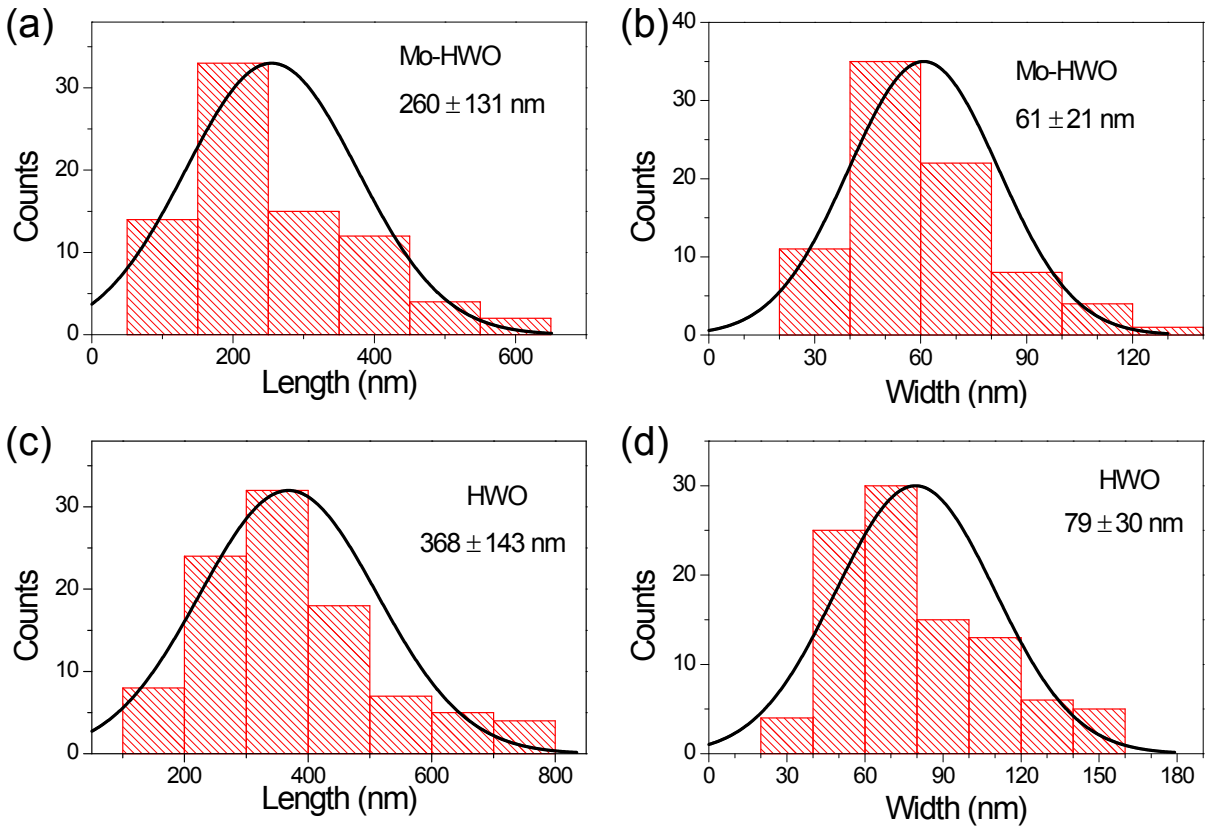

Fig. S4 Length and width distributions of the Mo-HWO (a,b) and HWO (c,d) nanorods counted from the TEM images.

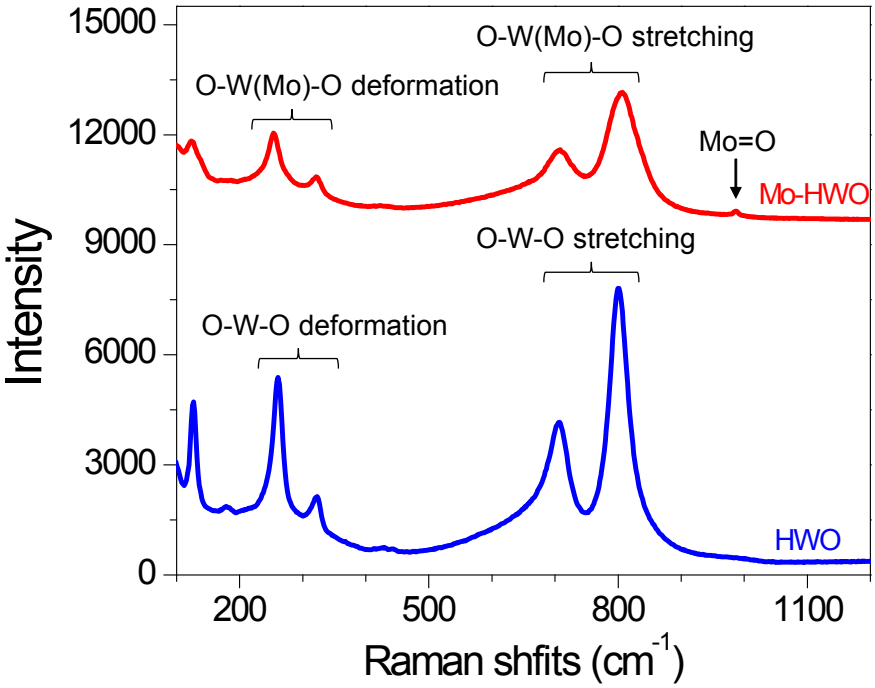

Fig. S5 Raman spectra of HWO and Mo-HWO.

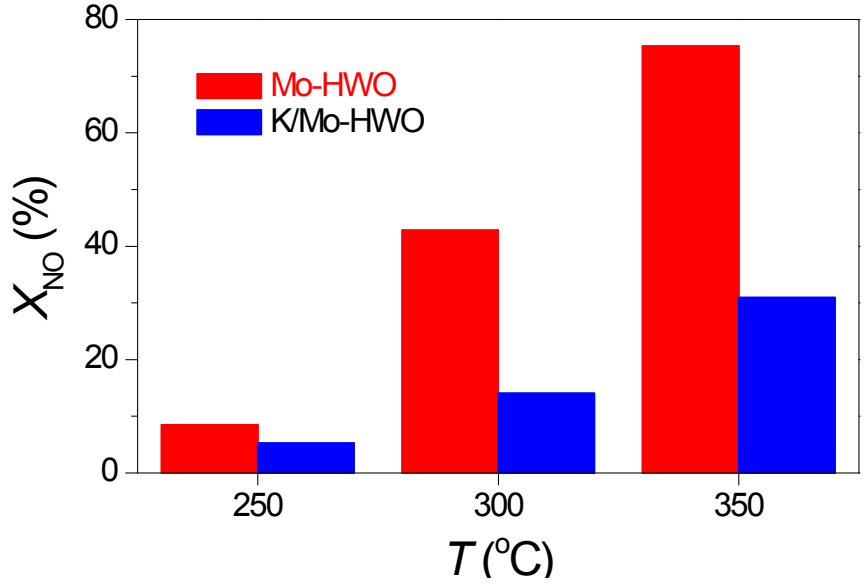

Fig. S6 The X_{NO} of Mo-HWO and HWO at different reaction temperature. Reaction conditions: 500 ppm NO, 500 ppm NH_3, 3.0 vol.% O_2, and balanced N_2, catalyst 0.5 g, gas flow rate 1,000 mL min^{-1}.

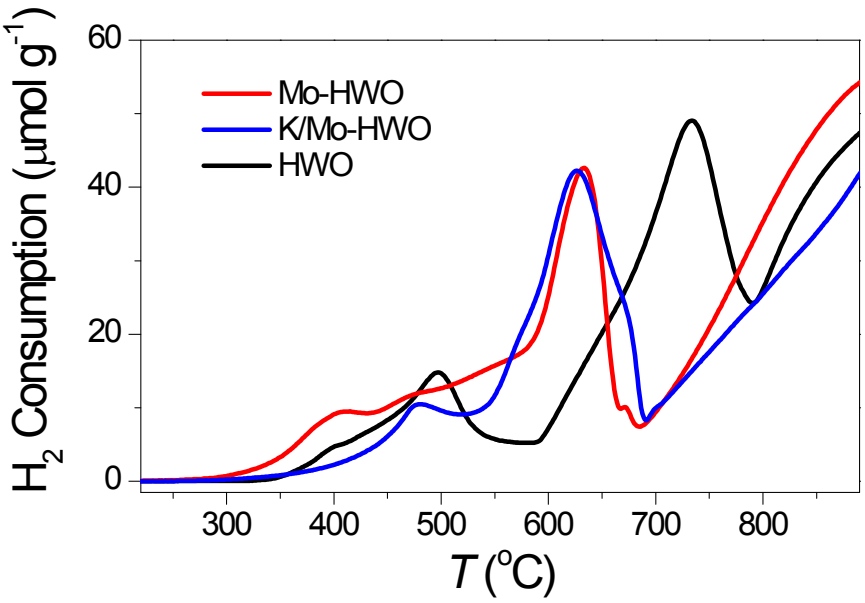

Fig. S7 H_2-TPR profiles of HWO, Mo-HWO and K/Mo-HWO.

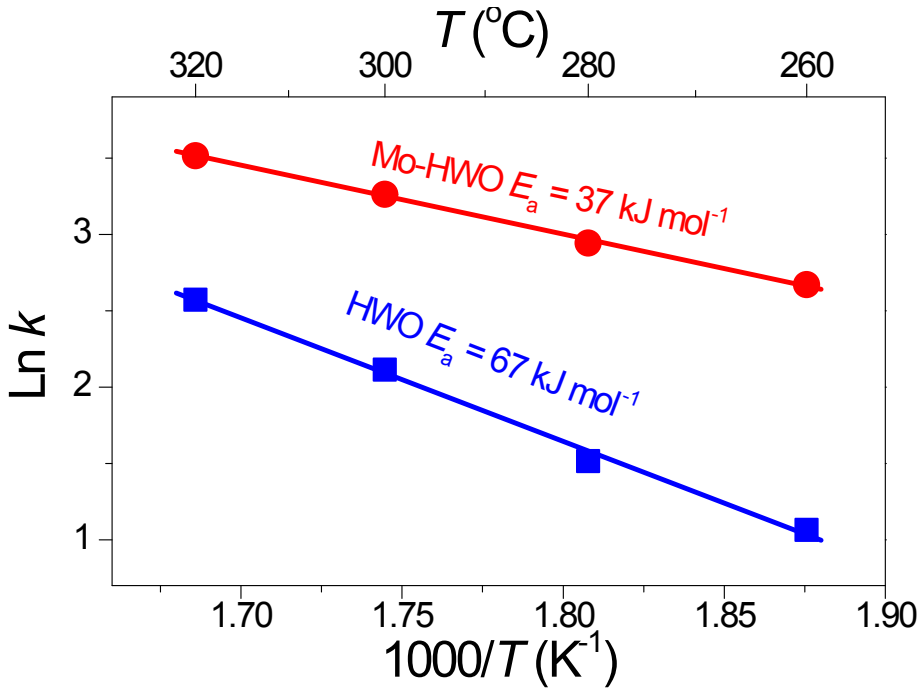

Fig. S8 Arrhenius plots of the samples at 260-320 °C.

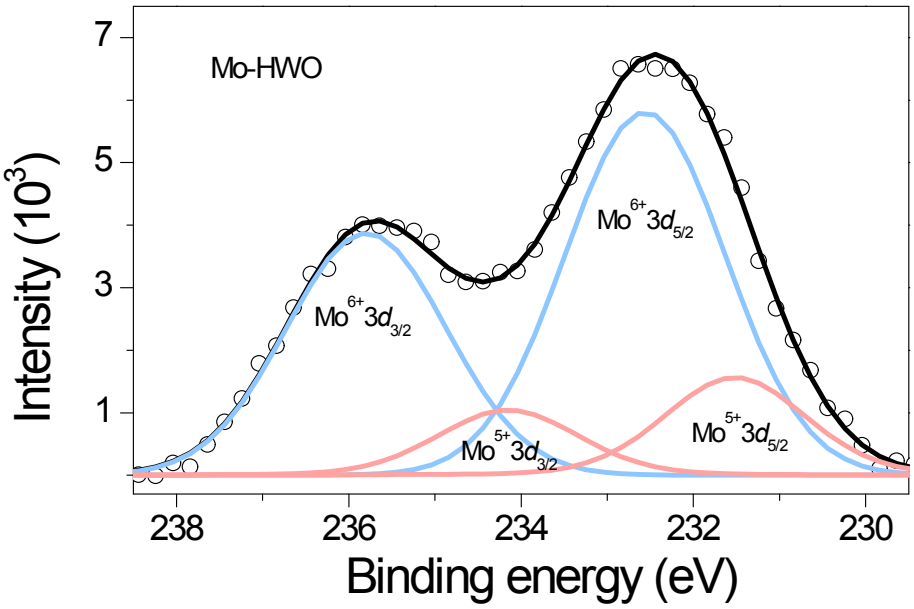

Fig. S9 Mo 3*d* XPS of Mo-HWO.