

## Supporting Information

### **Inhibitory role of excessive NH<sub>3</sub> in NH<sub>3</sub>-SCR on CeWO<sub>x</sub> at low temperatures**

Kuo Liu<sup>a,b</sup>, Yanlong Huo<sup>a,d</sup>, Zidi Yan<sup>a,d</sup>, Wenpo Shan<sup>c\*</sup>, Hong He<sup>a,c,d\*</sup>

<sup>a</sup> State Key Joint Laboratory of Environment Simulation and Pollution Control, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

<sup>b</sup> Editorial Office of Journal of Environmental Sciences, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

<sup>c</sup> Center for Excellence in Regional Atmospheric Environment, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China

<sup>d</sup> University of Chinese Academy of Sciences, Beijing 100049, China

\*Corresponding authors.

Fax: +86 10 62849123; Tel: +86 10 62849123;

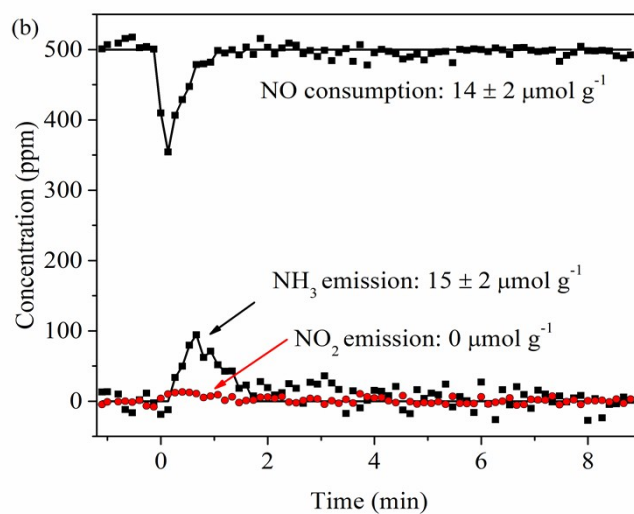
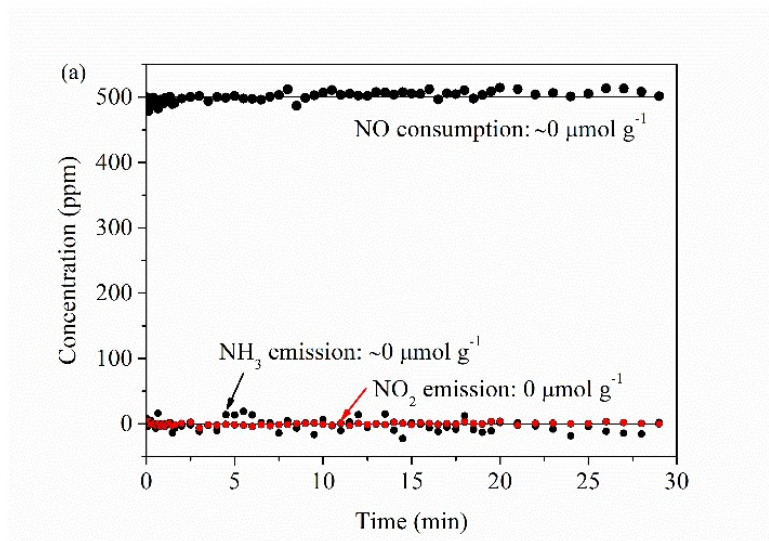
E-mails: wpshan@iue.ac.cn (W. Shan); honghe@rcees.ac.cn (H. He)

## S1 Experimental

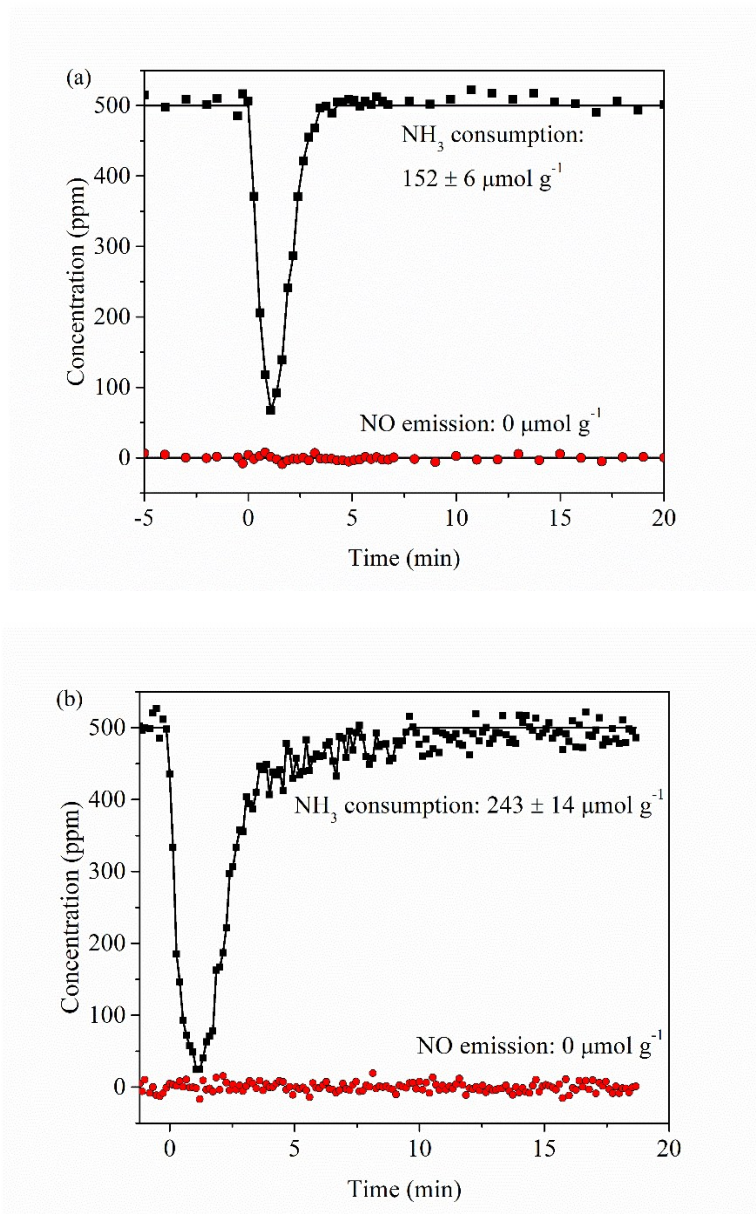
A homogeneous precipitation method was applied to prepare  $\text{CeWO}_x$  (Ce:W molar ratio 1:1), as reported in the literature.<sup>1</sup> In brief, an aqueous solution of ammonium tungstate ( $(\text{NH}_4)_{10}\text{W}_{12}\text{O}_{41}$ ), oxalic acid ( $\text{H}_2\text{C}_2\text{O}_4$ ), cerium nitrate ( $\text{Ce}(\text{NO}_3)_3$ ), and urea was stirred vigorously, and then heated overnight, followed by filtration, washing, drying and calcination.

The adsorption amounts of  $\text{NH}_3$  and  $\text{NO}$  were studied by a transient response method (TRM) quantitatively at room temperature as described in our previous studies.<sup>2,3</sup> Standard and fast SCR activities were tested at atmospheric pressure in a quartz flow reactor as described in a previous report,<sup>1</sup> applying 100 mg  $\text{CeWO}_x$  (40~60 mesh). The reaction conditions were: flow rates  $500 \text{ mL min}^{-1}$ , 500 ppm  $\text{NO}$ , 500 ppm or 1000 ppm  $\text{NH}_3$ , 5 vol.%  $\text{O}_2$ , 5%  $\text{H}_2\text{O}$  (when used) and balance  $\text{N}_2$  for standard SCR, and 250 ppm  $\text{NO}$ , 250 ppm  $\text{NO}_2$ , 500 ppm or 1000 ppm  $\text{NH}_3$ , 5 vol.%  $\text{O}_2$ , 5%  $\text{H}_2\text{O}$  (when used) and balance  $\text{N}_2$  for fast SCR.  $\text{NH}_3$ ,  $\text{NO}_2$ ,  $\text{NO}$ , and  $\text{N}_2\text{O}$  in the effluent gas were determined by a NEXUS 670-FTIR spectrometer quantitatively. The data were recorded under steady state and the  $\text{NO}_x$  conversion percentages were calculated based on the following equation:<sup>4</sup>

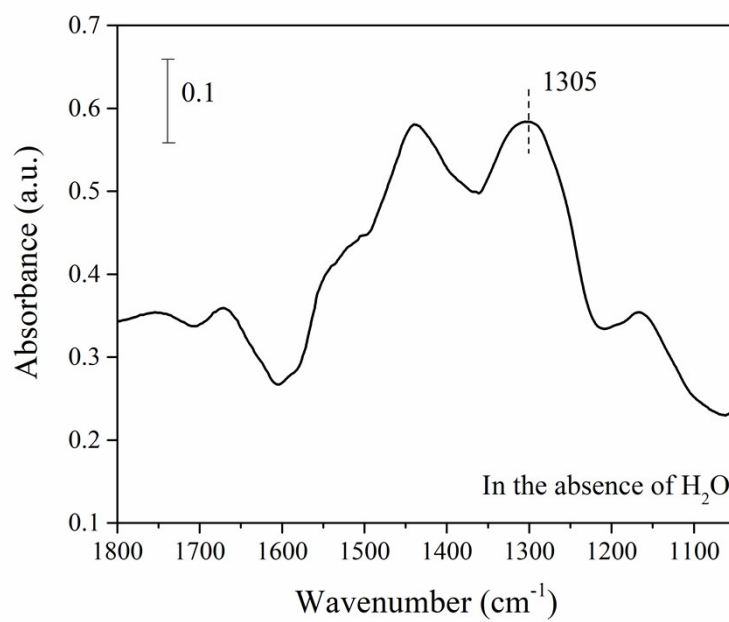
$$\text{NO}_x \text{ conversion} = \left( 1 - \frac{[\text{NO}]_{\text{out}} + [\text{NO}_2]_{\text{out}}}{[\text{NO}]_{\text{in}} + [\text{NO}_2]_{\text{in}}} \right) \times 100$$



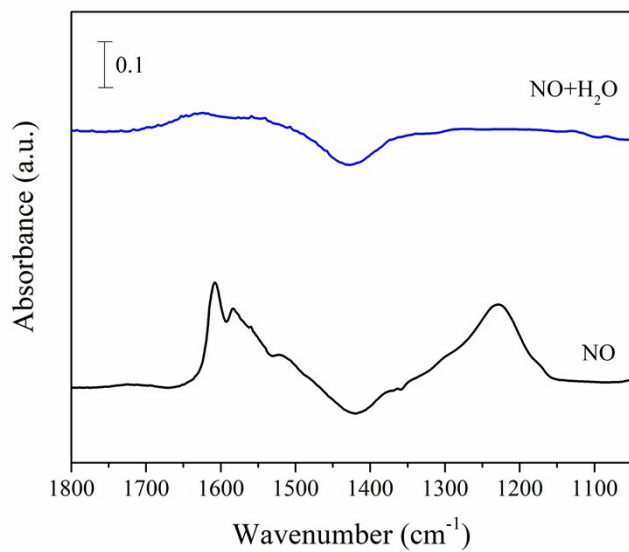
**Figure S1** (a) NO adsorption at room temperature over  $\text{CeWO}_x$  pre-treated in flowing 500 ppm  $\text{NH}_3$  in  $\text{N}_2$  until saturation and then purged by  $\text{N}_2$ , and (b) NO and 2 vol.%  $\text{H}_2\text{O}$  adsorption at room temperature over  $\text{CeWO}_x$  pre-treated in 2 vol.%  $\text{H}_2\text{O}$  and then flowing 500 ppm  $\text{NH}_3$  in  $\text{N}_2$  until saturation and then purged by  $\text{N}_2$ .



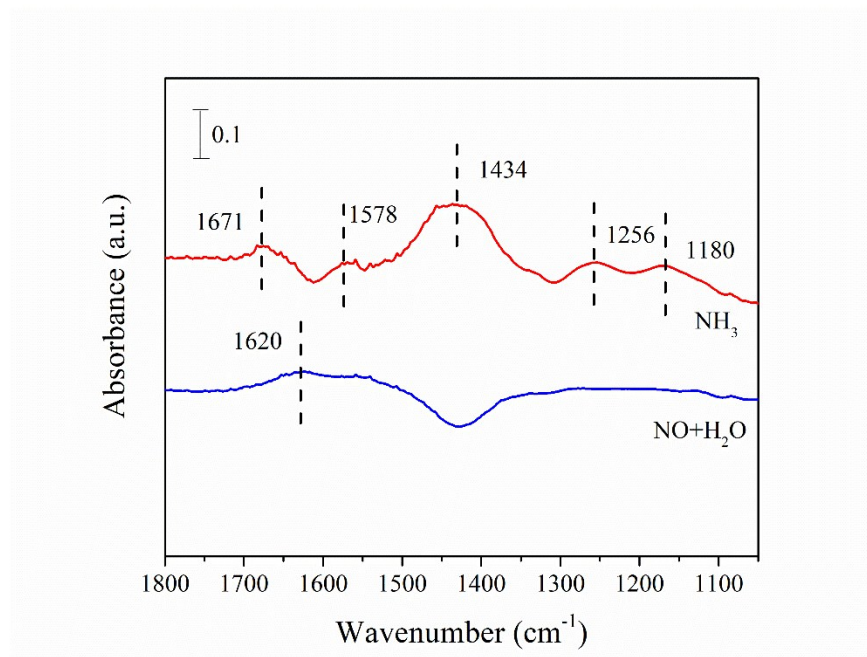
**Figure S2** NH<sub>3</sub> adsorption at room temperature over CeWO<sub>x</sub> pre-treated (a) in flowing 500 ppm NO in N<sub>2</sub> until saturation and then purged by N<sub>2</sub> and (b) in flowing 500 ppm NO and 2 vol% H<sub>2</sub>O in N<sub>2</sub> until saturation and then purged by N<sub>2</sub>.



**Figure S3** In situ DRIFTS results of 500 ppm NO-pretreated CeWO<sub>x</sub> treated by NH<sub>3</sub> at 30 °C.



**Figure S4** In situ DRIFTS results of CeWO<sub>x</sub> treated in 500 ppm NO and 500 ppm NO + 2 vol.% H<sub>2</sub>O after N<sub>2</sub> purge, respectively, at 150 °C.



**Figure S5** In situ DRIFTS results of  $\text{CeWO}_x$  treated in 500 ppm  $\text{NO} + 2 \text{ vol.}\% \text{H}_2\text{O}$  at  $150 \text{ }^\circ\text{C}$ , and then treated in 500 ppm  $\text{NH}_3$ .

**Table S1** NO and NH<sub>3</sub> adsorption at room temperature over CeWO<sub>x</sub>

	NH <sub>3</sub> adsorption ( $\mu\text{mol g}^{-1}$ )	NO adsorption after NH <sub>3</sub> adsorption ( $\mu\text{mol g}^{-1}$ )	NO adsorption ( $\mu\text{mol g}^{-1}$ )	NH <sub>3</sub> adsorption after NO adsorption ( $\mu\text{mol g}^{-1}$ )
In the absence of H <sub>2</sub> O	$160 \pm 5^a$	$\sim 0$	$\sim 10 \pm 2^a$	$\sim 152 \pm 6$
In the presence of H <sub>2</sub> O	$245 \pm 6^a$	$\sim 14 \pm 2$	$\sim 20 \pm 3^a$	$\sim 243 \pm 14$

<sup>a</sup> data from the literature.<sup>2</sup>**References:**

1. W.P. Shan, F.D. Liu, H. He, X.Y. Shi and C.B. Zhang, *Chem. Commun.* 2011, **47**, 8046-8048.
2. K. Liu, H. He, Y.B. Yu, Z.D. Yan, W.W. Yang and W.P. Shan, *J. Catal.* 2019, **369**, 372-381.
3. K. Liu, Z.D. Yan, H. He, Q.C. Feng and W.P. Shan, *Catal. Sci. Technol.* 2019, **9**, 5593-5604.
4. K. Liu, F.D. Liu, L.J. Xie, W.P. Shan and H. He, *Catal. Sci. Technol.* 2015, **5**, 2290-2299.