

## Supplementary Information

### **Efficient and stable low-temperature CO oxidation over Pt/In-SnO<sub>2</sub> composite triggered by abundant oxygen vacancies and adsorption sites**

Yukun Sun<sup>a,b,†</sup>, Yang Gao<sup>c,†</sup>, Chi He<sup>b,\*</sup>, Weiyu Song<sup>c</sup>, Zeyu Jiang<sup>b</sup>, Reem Albilali<sup>d</sup>, Bo Bai<sup>a,e,f,\*</sup>

<sup>a</sup>*Key Laboratory of Subsurface Hydrology and Ecological Effects in Arid Region, Ministry of Education, School of Water and Environment, Chang'an University, Xi'an 710064, P.R. China*

<sup>b</sup>*State Key Laboratory of Multiphase Flow in Power Engineering, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, P.R. China*

<sup>c</sup>*State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, P.R. China*

<sup>d</sup>*Department of Chemistry, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam 31441, Saudi Arabia*

<sup>e</sup>*Key Laboratory of Tibetan Medicine Research, Northwest Institute of Plateau Biology, Chinese Academy of Sciences, Xining 810008, P.R. China*

<sup>f</sup>*Qinghai Provincial Key Laboratory of Tibetan Medicine Research, Xining 810001, P.R. China*

<sup>†</sup>These authors contributed equally to this work.

To whom correspondence should be addressed:

Tel./Fax: +86 29 82663857; E-mail: chi\_he@xjtu.edu.cn (C. He)

Tel.: +86 29 82339052; Fax: +86 29 82339961; E-mail: baibochina@163.com (B. Bai)

## Supplementary Information

### Experimental

#### Material characterizations

The specific surface area and pore structure of prepared materials was analyzed at 77 K on a Tristar 3000 analyzer. The samples were degassed at 300 °C for 2 h before the adsorption measurements. X-ray diffraction (XRD) experiments were performed by using the Ni-filtered Cu K $\alpha$  radiation from a highly stabilized and automated PAN-analytical X-ray generator operated at 40 kV and 40 mA. The X-ray generator was coupled with a PW3071/60 Bracket goniometer to mount the sample. Step-scan data obtained with a step size of 0.02° and a counting time of 2 s per step were recorded in 2 $\theta$  range of 20-80°. The morphology and micro-feature of obtained samples was characterized by scanning electron microscopy (SEM; S-4800) and transmission electron microscopy (TEM; JEOL 2100F) equipped with an energy-dispersive X-ray (EDX) detector. The Raman spectra were collected at room temperature on a Thermo Scientific DXR Raman microscope using a heliumneon laser with an excitation wavelength of 532 nm (laser power 10 mW). X-ray photoelectron spectroscopy (XPS; Kratos-ULTRA AXIS DLD) was used to determine the surface state of prepared materials. Binding energies of all elements were calibrated relative to the adventitious carbon with C1s at 284.8 eV. All the data were analyzed by XPSPEAK software using Shirley type background. The Pt dispersion was tested by CO pulse on a Micromecitics AutoChem II 2920 chemisorption analyzer. The catalyst (100 mg) were placed in a U-shaped quartz reactor and pretreated with 5 vol.% H<sub>2</sub>/Ar at 400 °C for 60 min. After cooling to 25 °C, 1 vol.% CO/He (50 mL min<sup>-1</sup>) was injected into the sample cell every two minutes until CO signal was kept constant. The temperature-programmed reduction (H<sub>2</sub>-TPR) was performed on a Chem BET-3000 (Quanta chrome Instruments). Typically, 100 mg of sample

## Supplementary Information

was loaded in a U-type quartz reactor and pretreated in a flow of N<sub>2</sub> (100 mL min<sup>-1</sup>) at 300 °C for 1 h to remove adsorbed water and other impurities. The sample was then cooled down to room temperature in a flow of nitrogen and then heated from room temperature to 950 °C with a ramp rate of 10 °C min<sup>-1</sup>. The signals of thermal conductivity detector (TCD) were qualitatively calibrated using high-purity CuO (Sigma Aldrich) with an assumption of stoichiometric reduction of CuO by H<sub>2</sub>.

### Catalytic performance

Catalytic oxidation of CO was carried out in a fixed-bed quartz tube reactor (4 mm inner diameter) with a ramp rate of 2 °C min<sup>-1</sup>. The catalyst temperature was electronically controlled and measured by two K-type thermocouples located upstream and downstream of the catalyst bed. 50 mg of catalyst was placed in the reactor and a gas mixture containing 1% CO and 20% O<sub>2</sub>/N<sub>2</sub> was fed. The main gas lines were wrapped by heating tapes and isolation materials to maintain the downstream lines isothermal at 120 °C before the FTIR gas analyzer. The total flow rate for all tests was fixed at 100 mL min<sup>-1</sup> (WHSV of 120,000 mL g<sup>-1</sup> h<sup>-1</sup>). An Antaris™ IGS Gas Analyzer (Thermo Fisher) was used to analyze the gas reactants and products.

The conversion of CO is defined by Eq. (1):

$$X_{\text{CO}} = \frac{[C_{\text{CO}}]_{\text{in}} - [C_{\text{CO}}]_{\text{out}}}{[C_{\text{CO}}]_{\text{in}}} \times 100\% \quad (1)$$

where  $[C_{\text{CO}}]_{\text{in}}$  and  $[C_{\text{CO}}]_{\text{out}}$  represent the inlet and outlet CO concentrations, respectively.

The reaction rate was tested using 50 mg of catalyst in the feed gas of 1 vol.% CO + 20 vol.% O<sub>2</sub> + 79 vol.% N<sub>2</sub> with WHSV of 120,000 mL g<sup>-1</sup> h<sup>-1</sup>. The reaction rate of CO oxidation ( $r_{\text{CO}}$ ) over prepared catalysts was calculated using the following equations:

## Supplementary Information

$$r_{\text{CO, Pt}}(\text{mol g}^{-1} \text{s}^{-1}) = \frac{[X_{\text{CO}}][V_{\text{CO}}]}{[m_{\text{cat.}}][\omega_{\text{Pt}}]} \quad (2)$$

$$r_{\text{CO}}(\text{mol g}^{-1} \text{s}^{-1}) = \frac{[X_{\text{CO}}][V_{\text{CO}}]}{[m_{\text{cat.}}]} \quad (3)$$

where  $[C_{\text{CO}}]$  is the concentration of CO in the feed gas;  $[X_{\text{CO}}]$  is the conversion of CO;  $[V_{\text{CO}}]$  is the CO gas flow rate ( $\text{mol s}^{-1}$ );  $[m_{\text{cat.}}]$  is the mass of catalyst used;  $[\omega_{\text{Pt}}]$  is the Pt content on catalyst.

The turnover frequency (TOF) of CO oxidation on different catalysts was calculated using Eq. (4)<sup>1</sup>:

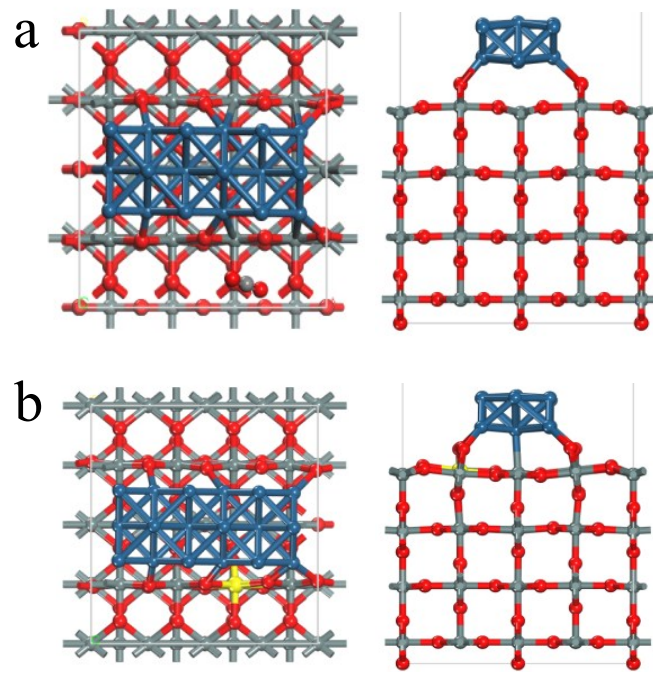
$$\text{TOF}_{\text{Pt}}(\text{s}^{-1}) = \frac{[r_{\text{CO}}][M_{\text{Pt}}]}{[D_{\text{Pt}}]} \quad (4)$$

where  $[M_{\text{Pt}}]$  is the atomic weight of Pt ( $195.078 \text{ g mol}^{-1}$ );  $[D_{\text{Pt}}]$  is the Pt dispersion, which is measured by CO chemical adsorption.

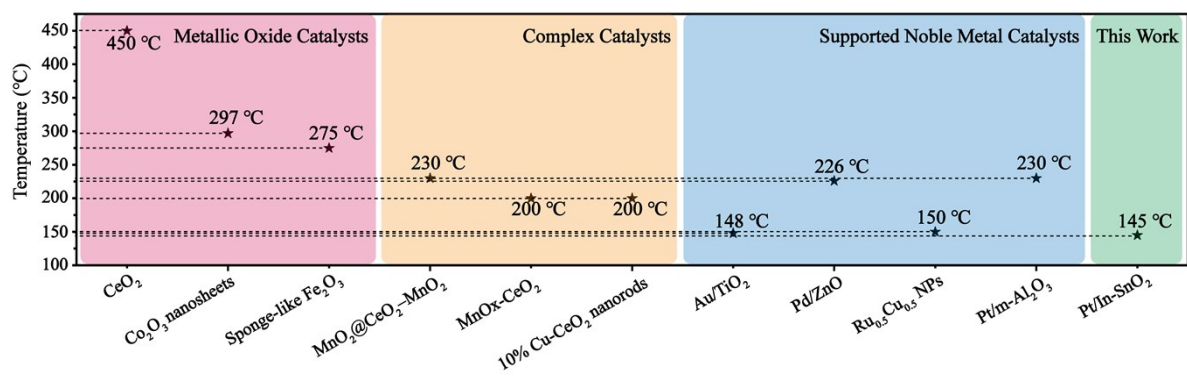
The temperature dependent reaction rate constant of chemical reactions can be interpreted in terms of the Arrhenius equation<sup>2</sup>:

$$k = Ae^{-E_a/RT} \quad (5)$$

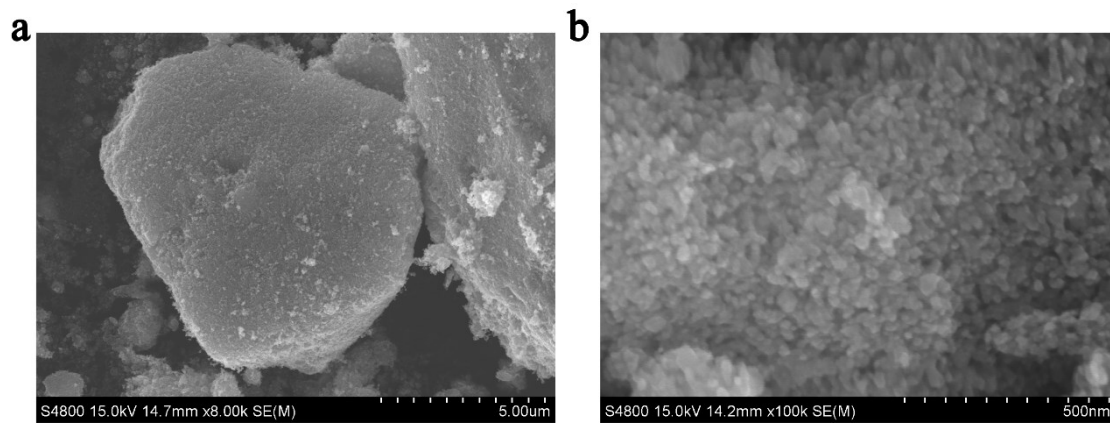
where  $k$  is the rate constant,  $A$  is the pre-exponential factor,  $E_a$  is the activation energy,  $R$  is molar gas constant, and  $T$  is the absolute temperature. The reaction rate can be expressed as Eq. (6) and then  $E_a$  can be obtained by plotting  $\ln k$  vs  $1000/T$ .



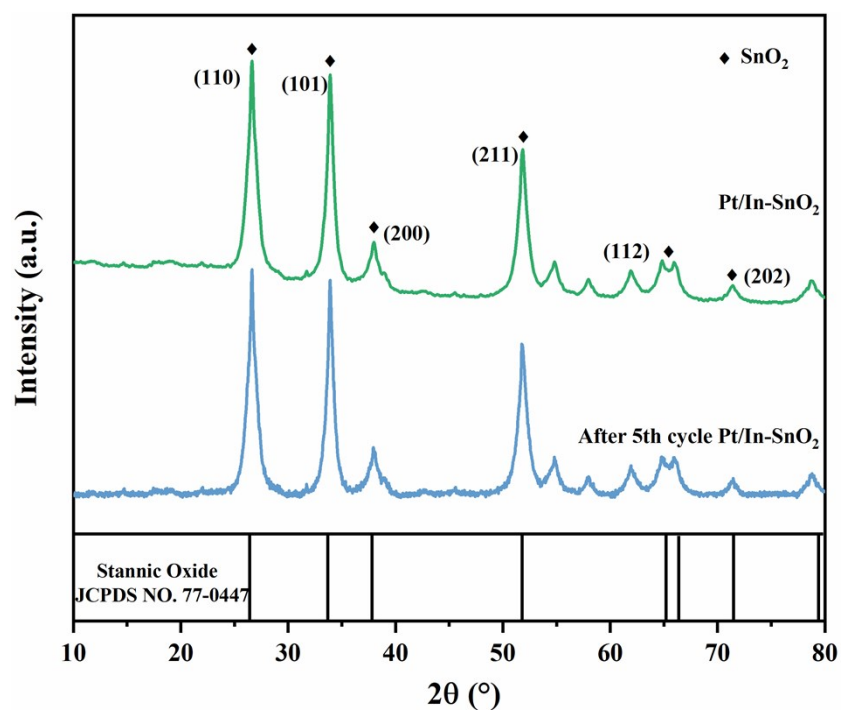
**Fig. S1** Top and side view of (a) Pt/SnO<sub>2</sub> (110) and (b) Pt/In-SnO<sub>2</sub> model.



**Fig. S2** Comparison of different catalysts reported for CO oxidation.

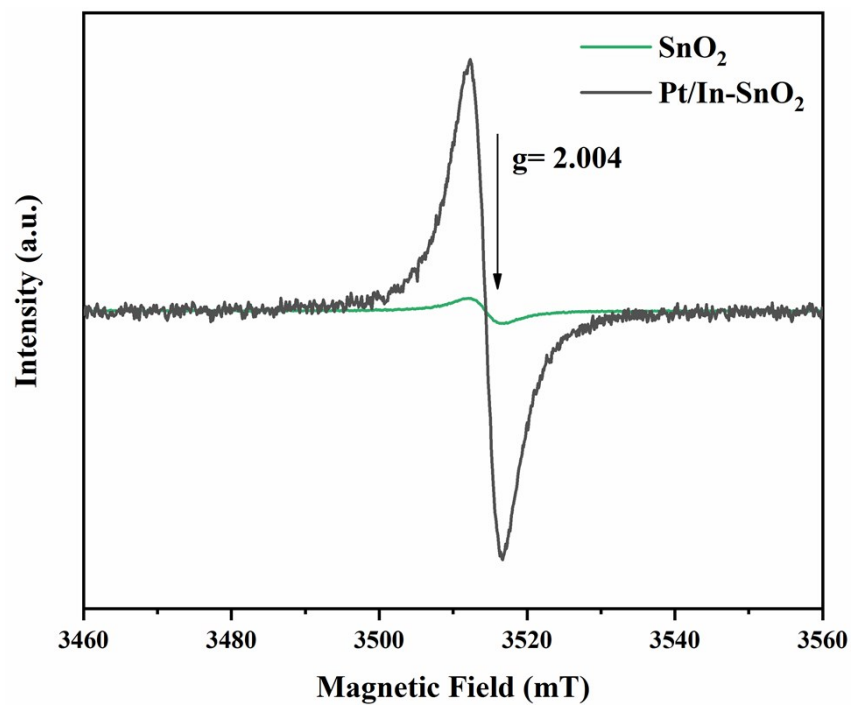


**Fig. S3** SEM images of Pt/In-SnO<sub>2</sub> catalyst after five cycles of CO oxidation.



**Fig. S4** XRD patterns of Pt/In-SnO<sub>2</sub> catalyst after five cycles of CO oxidation.





**Fig. S5** EPR spectrum of SnO<sub>2</sub> and Pt/In-SnO<sub>2</sub> catalysts.

**Table S1** Comparison of CO oxidation over Pt/In-SnO<sub>2</sub> and typical catalysts reported in the literature.

Catalyst	Gas mixture	Total flow rate (mL min <sup>-1</sup> )	WHSV (mL g <sup>-1</sup> h <sup>-1</sup> )	T <sub>100</sub> (°C)	References
MnO <sub>x</sub> -CeO <sub>2</sub>	2 vol% CO, 5 vol% O <sub>2</sub>	133	40,000	200	3
Co <sub>3</sub> O <sub>4</sub> nanosheets	1 vol.% CO, 20 vol.% O <sub>2</sub>	30	18,000	297	4
Sponge-like Fe <sub>2</sub> O <sub>3</sub>	1 vol.% CO, 10 vol.% O <sub>2</sub>	100	36,000	275	5
MnO <sub>2</sub> @CeO <sub>2</sub> -MnO <sub>2</sub>	0.8 vol.% CO, 2 vol.% O <sub>2</sub>	100	60,000	230	6
10%Cu-CeO <sub>2</sub> nanorods	1 vol.% CO, 20 vol.% O <sub>2</sub>	70	140,000	200	7
Au/TiO <sub>2</sub>	1 vol.% CO, 1 vol.% O <sub>2</sub>	60	20,000	148	8
Pd/ZnO	0.5 vol.% CO, 1 vol.% O <sub>2</sub>	100	240,000	226	9
Ru <sub>0.5</sub> Cu <sub>0.5</sub> NPs	1 vol.% CO, 1 vol.% O <sub>2</sub>	50	20,000	150	10
Pt/m-Al <sub>2</sub> O <sub>3</sub>	2.5 vol.% CO, 2.5 vol.% O <sub>2</sub>	80	48,000	230	11
Pt/In-SnO <sub>2</sub>	1 vol.% CO, 1.5 vol.% O <sub>2</sub>	100	120,000	145	This work

## References

- 1 Y. Ding, Q. Wu, B. Lin, Y. Guo, Y. Guo, Y. Wang, L. Wang, W. Zhan, *Appl. Catal. B: Environ.*, 2020, **266**, 118631.
- 2 Y. Cai, J. Xu, Y. Guo, J. Liu, *ACS Catal.*, 2019, **9**, 2558-2567.
- 3 C. Wang, C. Wen, J. Lauterbach, E. Sasmaz, *Appl. Catal. B: Environ.*, 2017, **206**, 1-8.
- 4 F. Wang, L. Zhang, L. Xu, Z. Deng, W. Shi, *Fuel*, 2017, **203**, 419-429.
- 5 W. Li, Y. Hu, H. Jiang, Y. Jiang, Y. Wang, S. Huang, P. Biswas, C. Li, *Appl. Surf. Sci.*, 2018, **44**, 763-771.
- 6 J. Zhang, Y. Cao, C. Wang, R. Ran, *ACS Appl. Mater. Inter.*, 2016, **8**, 8670-8677.
- 7 S. A. Mock, S. E. Sharp, T. R. Stoner, M. J. Radetic, E. T. Zell, R. Wang, *J. Colloid Interf. Sci.*, 2016, **466**, 261–267
- 8 H. Guan, J. Lin, B. Qiao, X. Yang, L. Li, S. Miao, J. Liu, A. Wang, X. Wang, T. Zhang, *Angew. Chem. Int. Ed.*, 2016, **55**, 2820-2824.
- 9 P. Kast, M. Friedricha, F. Girgsdies, J. Kröhnert, D. Teschner, T. Lunkenbeina, M. Behrens, R. Schlögl, *Catal. Today*, 2016, **206**, 21-31.
- 10 B. Huang, H. Kobayashi, T. Yamamoto, S. Matsumura, Y. Nishida, K. Sato, K. Nagaoka, S. Kawaguchi, Y. Kubota, H. Kitagawa, *J. Am. Chem. Soc.*, 2017, **139**, 4643–4646.
- 11 Z. Zhang, Y. Zhu, H. Asakura, B. Zhang, J. Zhang, M. Zhou, Y. Han, T. Tanaka, Aiqin Wang, T. Zhang, N. Yan, *Nat. Commun.*, 2017, **8**, 16100-16110.