

Supporting information for

**Design of interface structure to enhance the operational  
temperature range of CuO/Cu-SSZ-13 for concurrent NO<sub>x</sub> selective  
catalytic reduction and CO oxidation**

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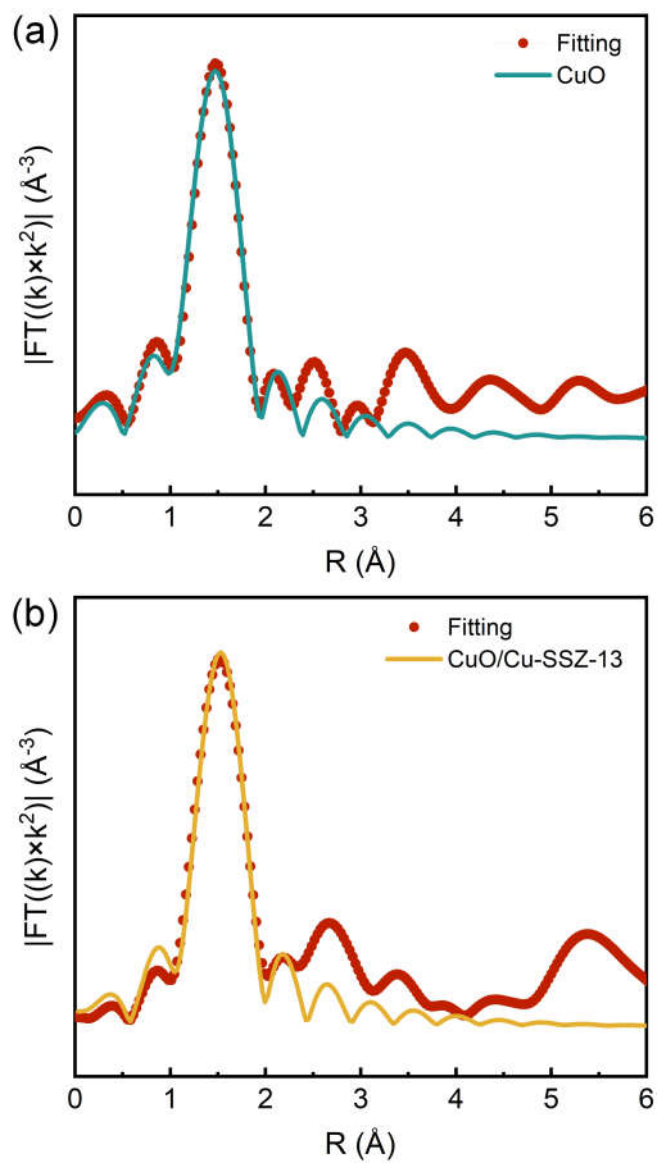
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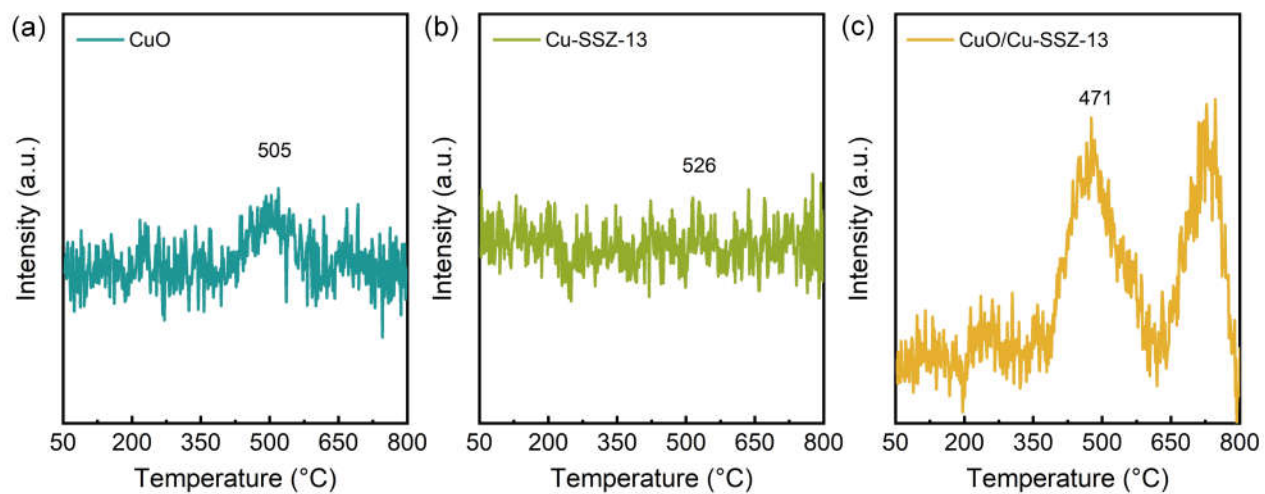
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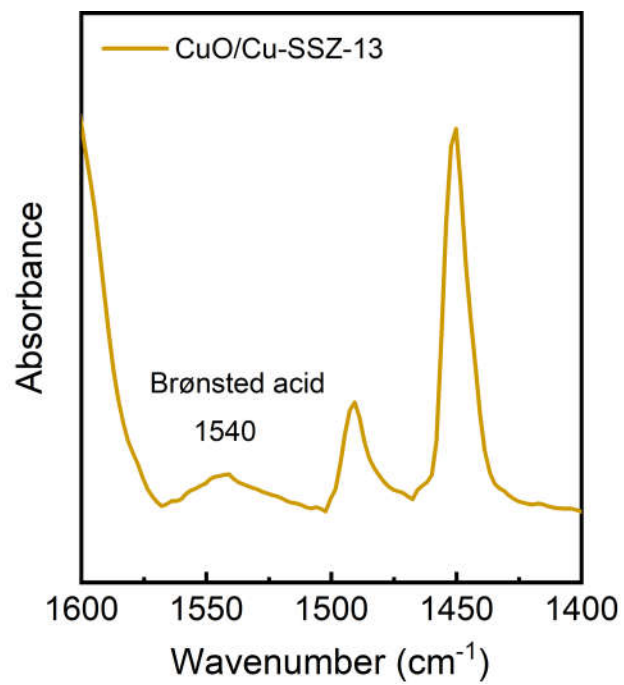
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Yue)



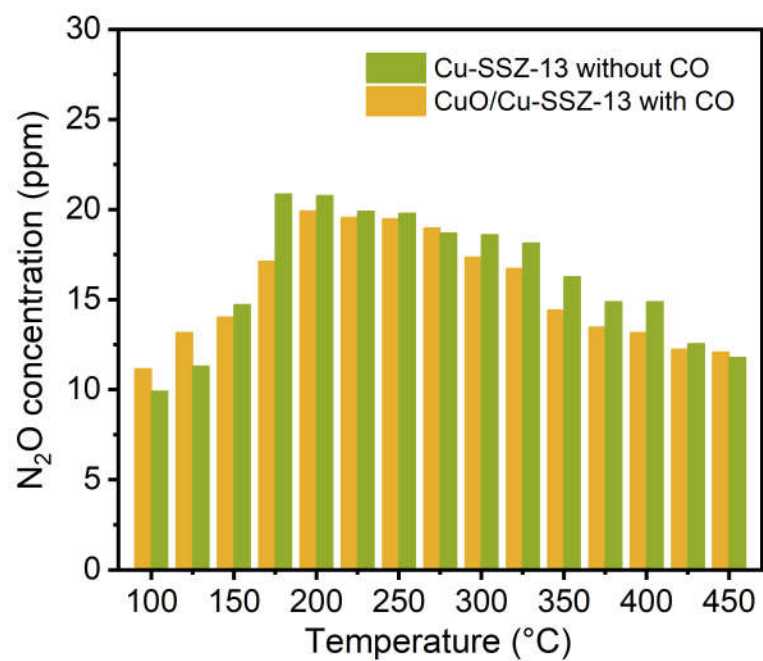
**Fig. S1** EXAFS fitting results of (a) self-prepared CuO and (b) CuO/Cu-SSZ-13.



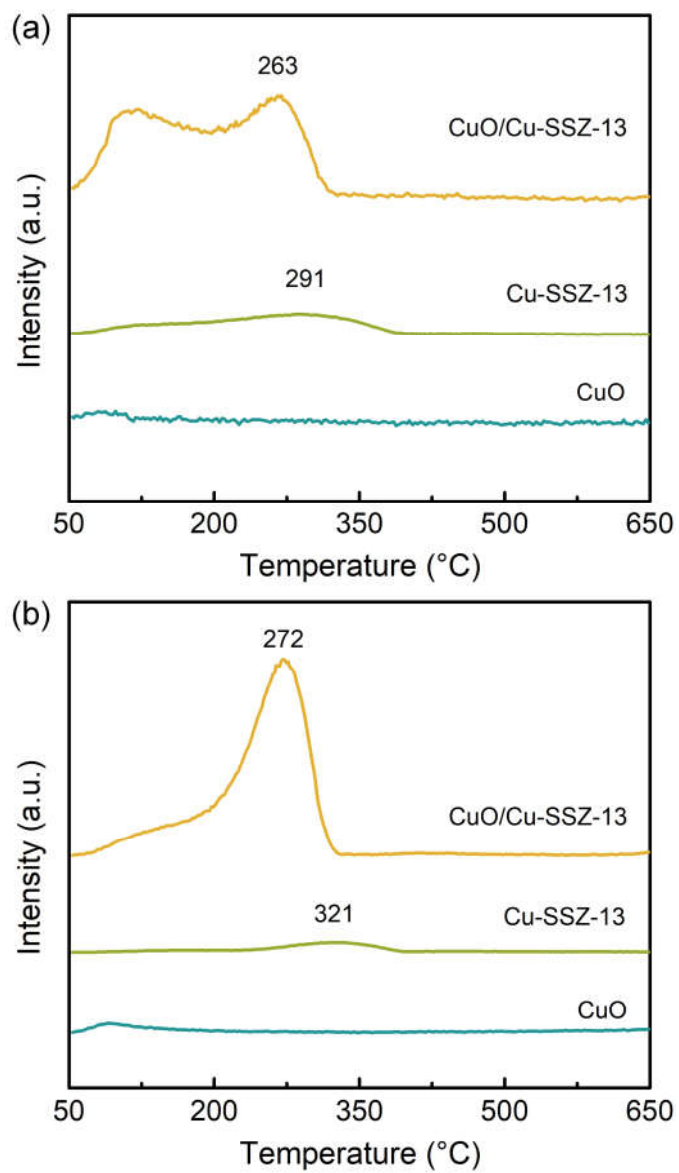
**Fig. S2** O<sub>2</sub>-TPD-MS curves of self-prepared (a) CuO, (b) Cu-SSZ-13 and (c) CuO/Cu-SSZ-13.



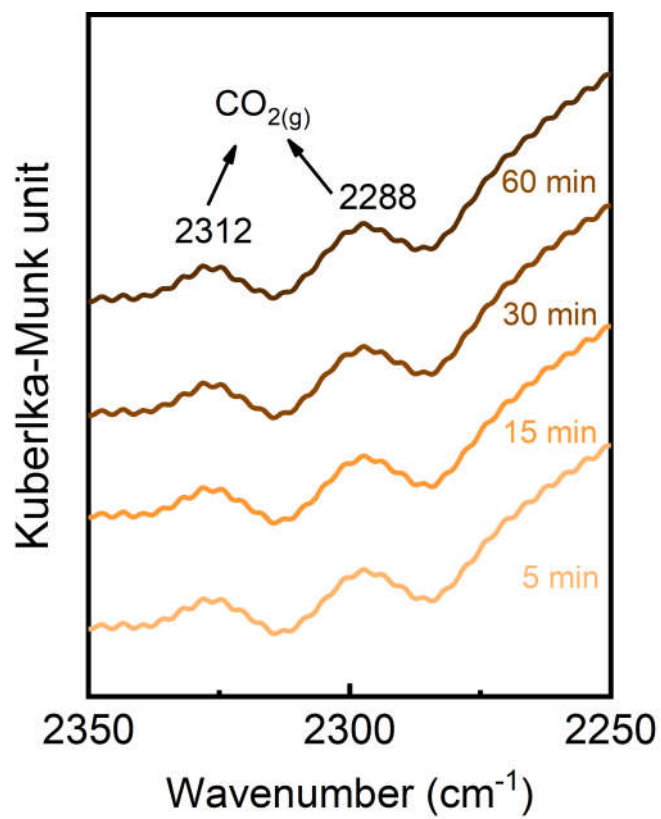
**Fig. S3** Py-FTIR spectra of CuO/Cu-SSZ-13 at 150 °C.



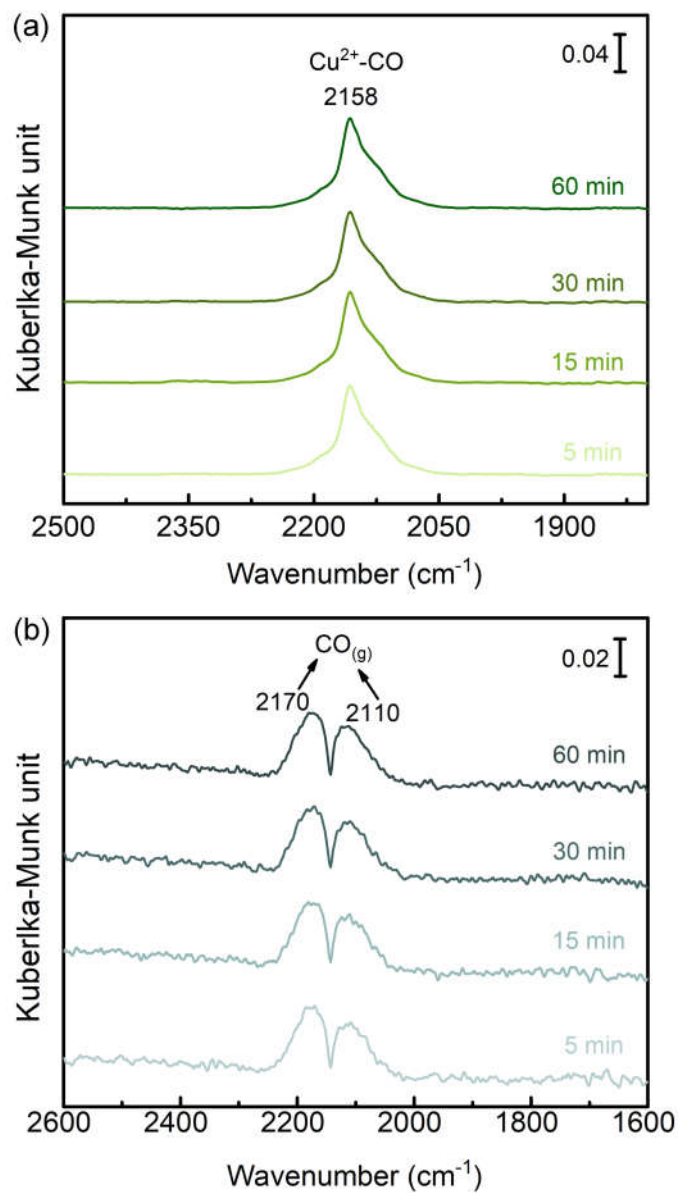
**Fig. S4** N<sub>2</sub>O concentration of Cu-SSZ-13 and CuO/Cu-SSZ-13.



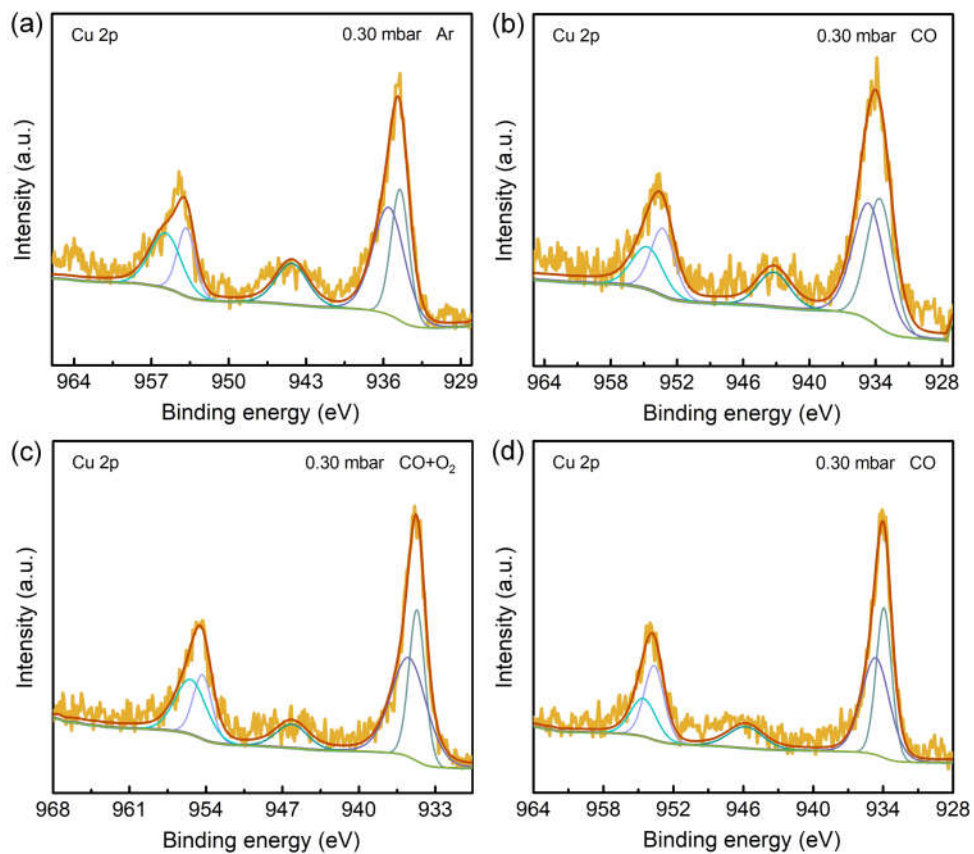
**Fig. S5** (a) CO and (b) CO<sub>2</sub> desorption curves of self-prepared CuO, Cu-SSZ-13 and CuO/Cu-SSZ-13 by CO-TPD-MS experiments.



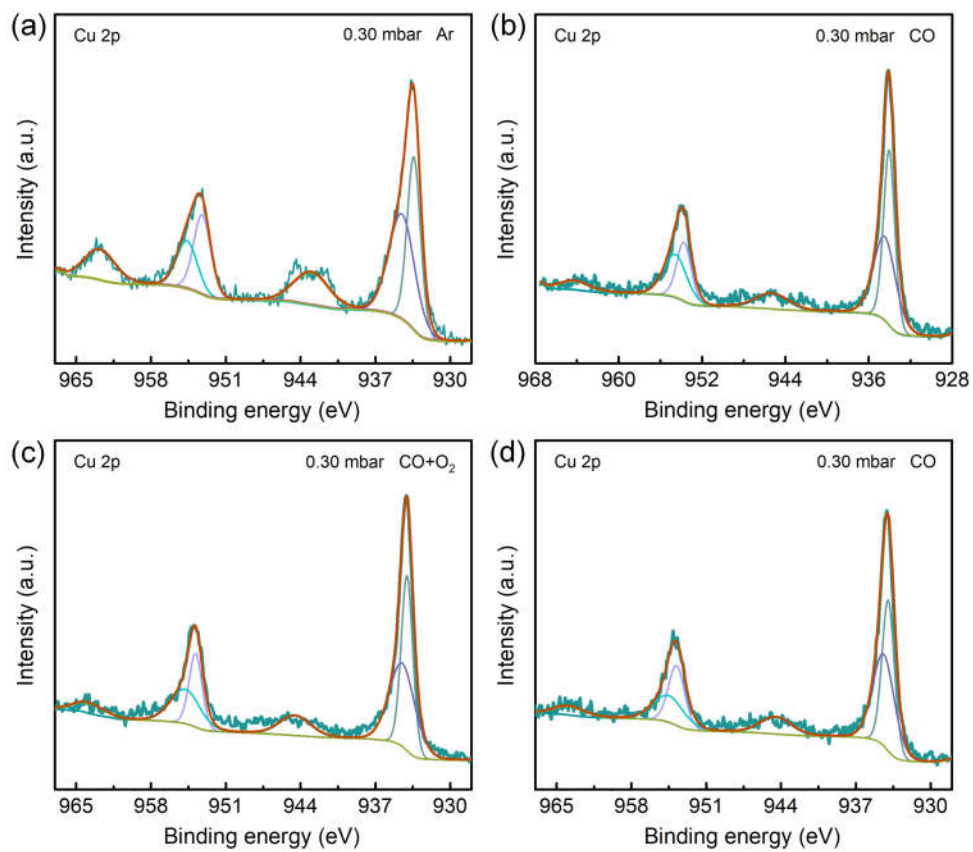
**Fig. S6** CO + O<sub>2</sub>-*in situ* DRIFTS spectra of CuO/Cu-SSZ-13 for 60 min at 200 °C.



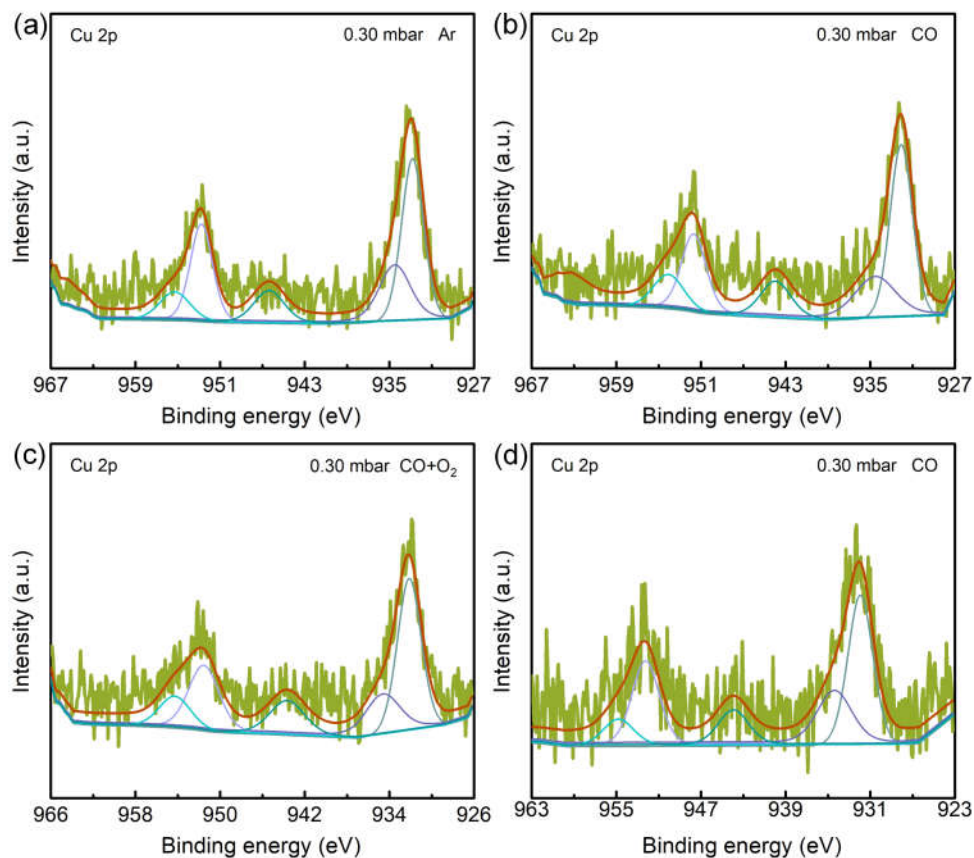
**Fig. S7** CO + O<sub>2</sub>-*in situ* DRIFTS spectra of (a) Cu-SSZ-13 and (b) CuO for 60 min at 200 °C.



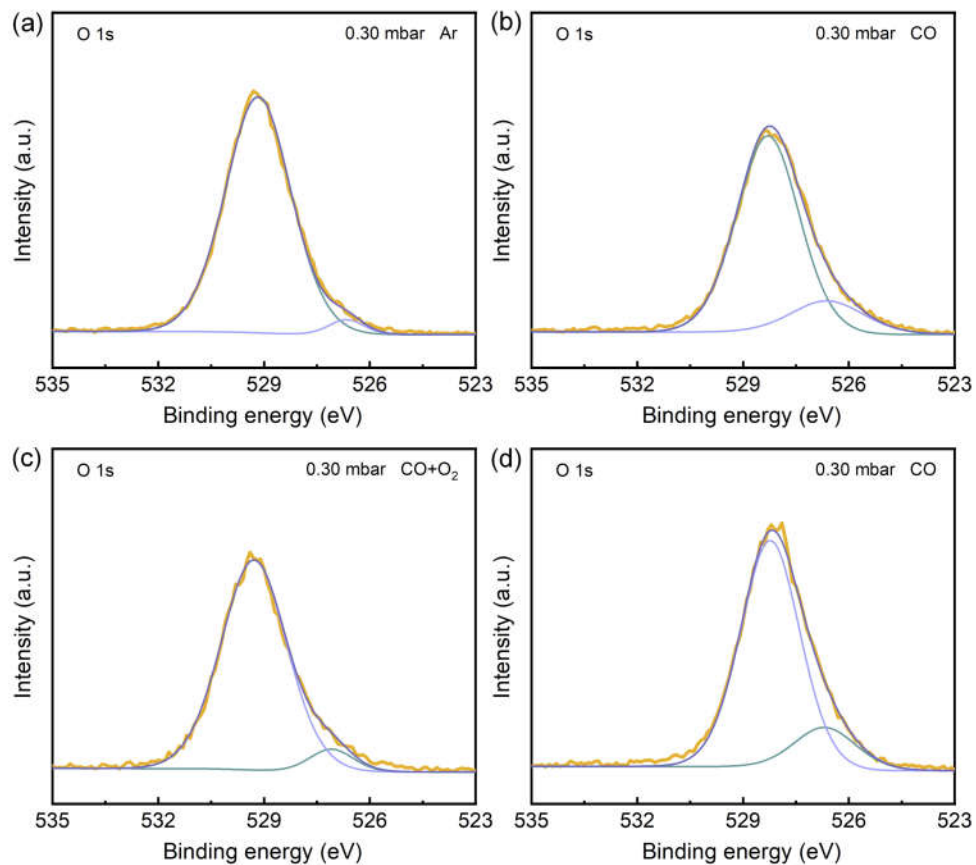
**Fig. S8** Cu 2p XPS spectra of CuO/Cu-SSZ-13 under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



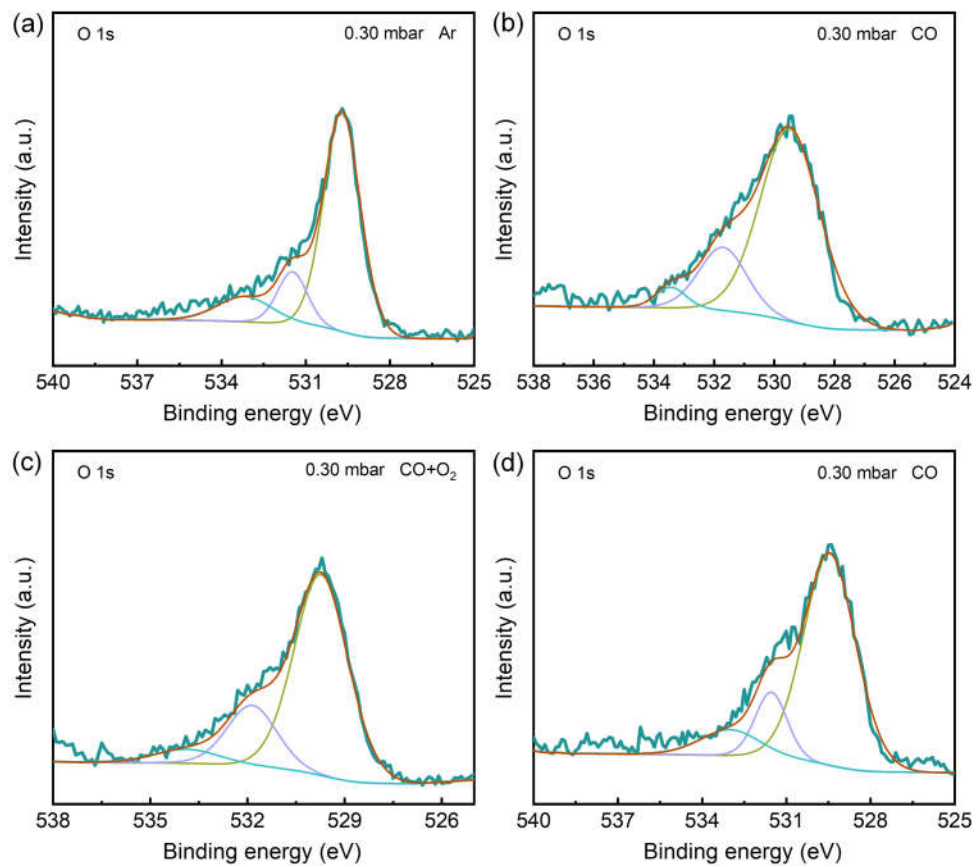
**Fig. S9** Cu 2p XPS spectra of CuO under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



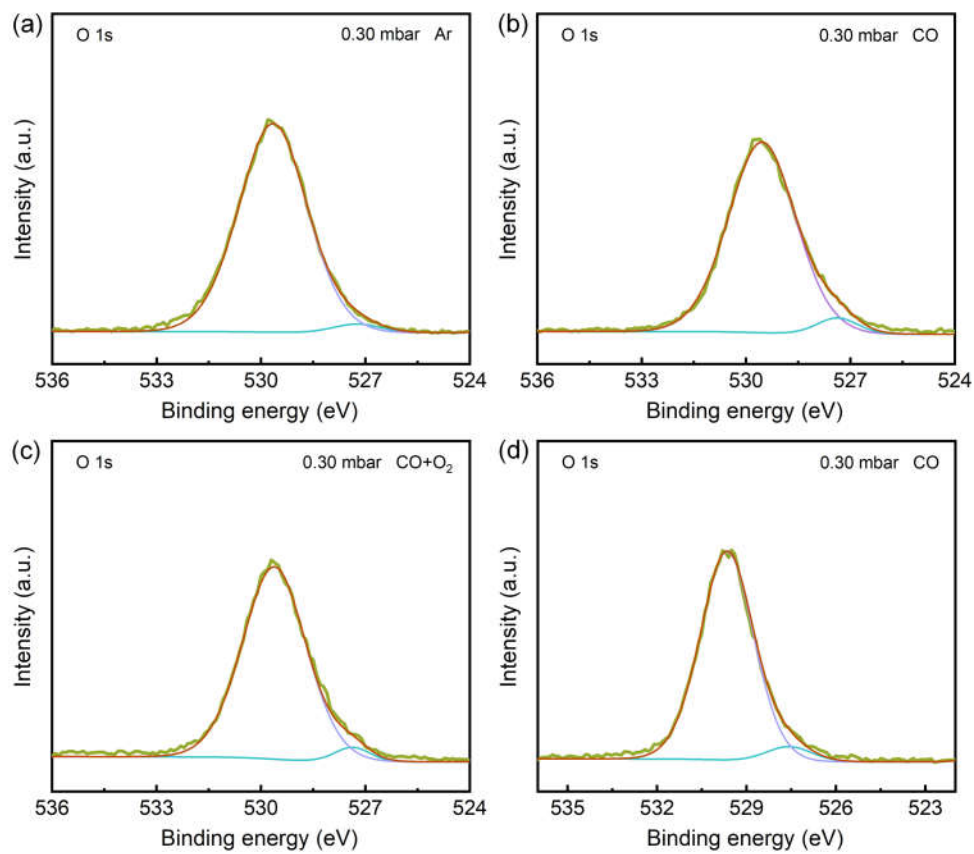
**Fig. S10** Cu 2p XPS spectra of Cu-SSZ-13 under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



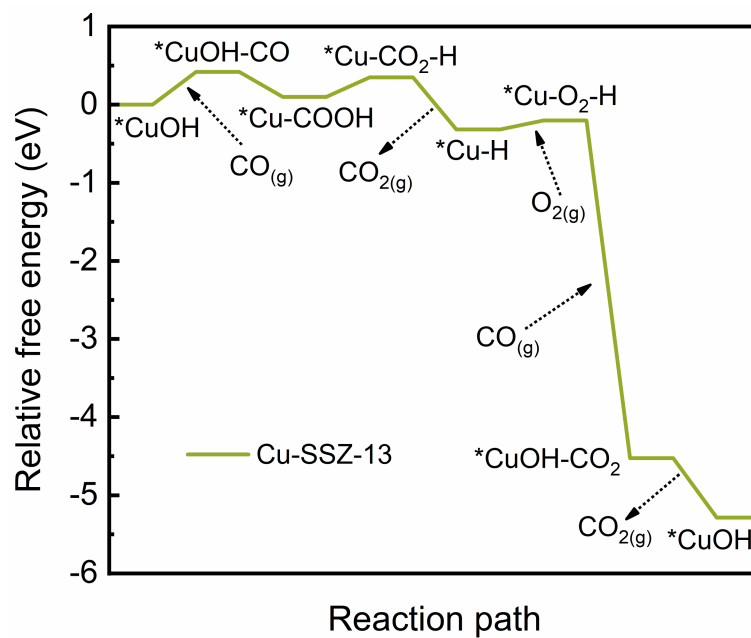
**Fig. S11** O 1s XPS spectra of CuO/Cu-SSZ-13 under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



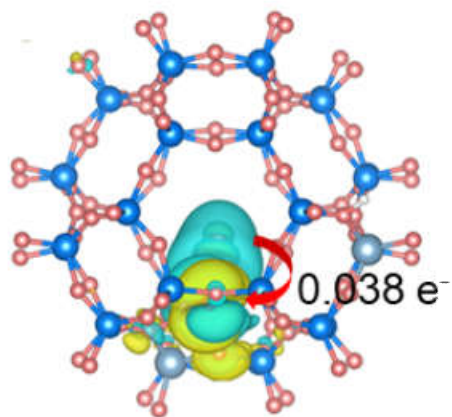
**Fig. S12** O 1s XPS spectra of CuO under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



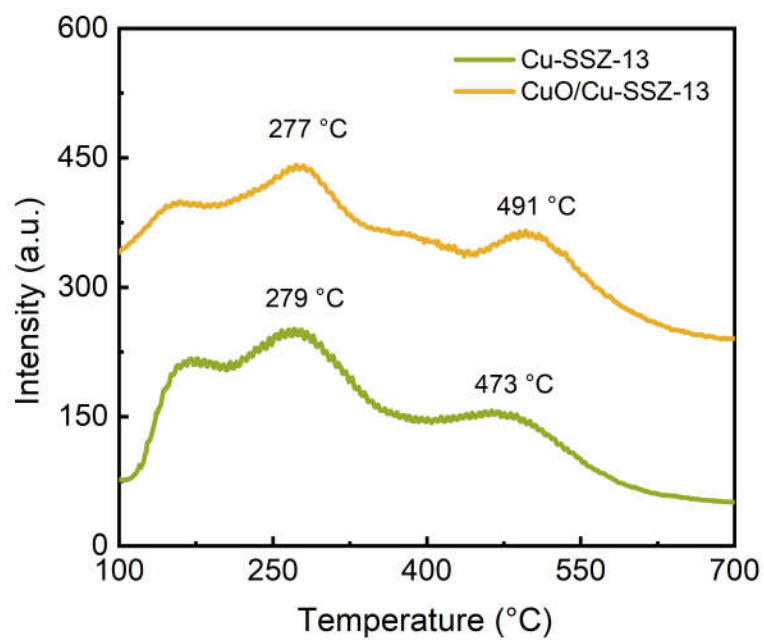
**Fig. S13** O 1s XPS spectra of Cu-SSZ-13 under (a) Ar, (b) CO, (c) CO + O<sub>2</sub> and (d) CO atmosphere at 200 °C.



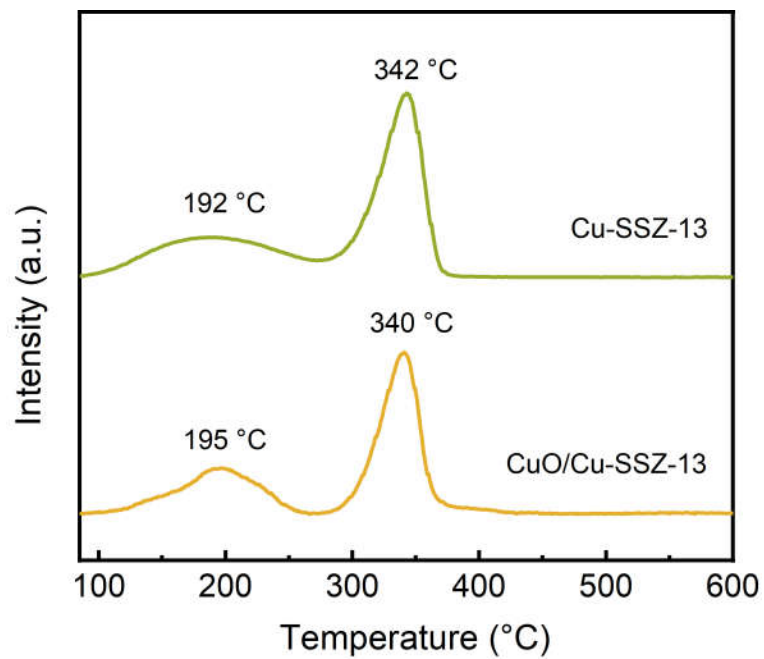
**Fig. S14** The free energy change diagram of the CO oxidation process over Cu-SSZ-13 at 200 °C.



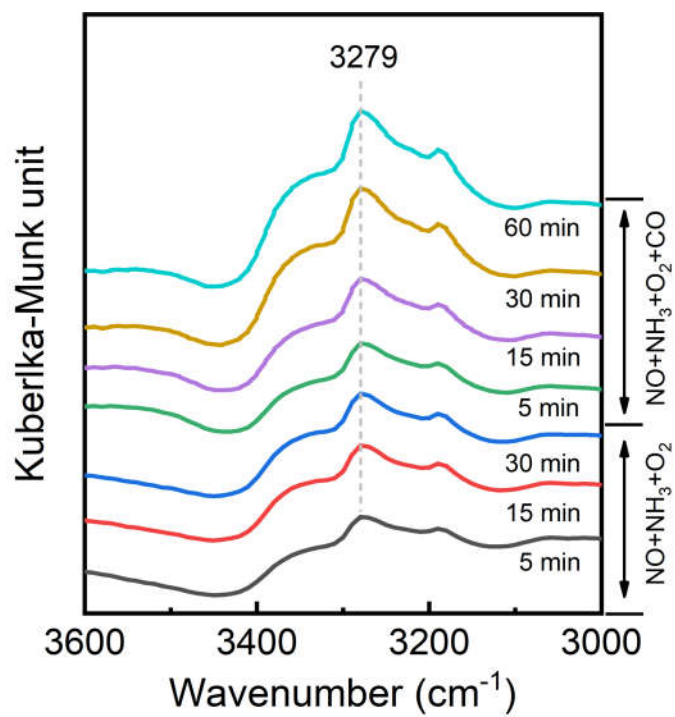
**Fig. S15** Charge density difference and Bader charge of Cu-SSZ-13 for CO adsorption.



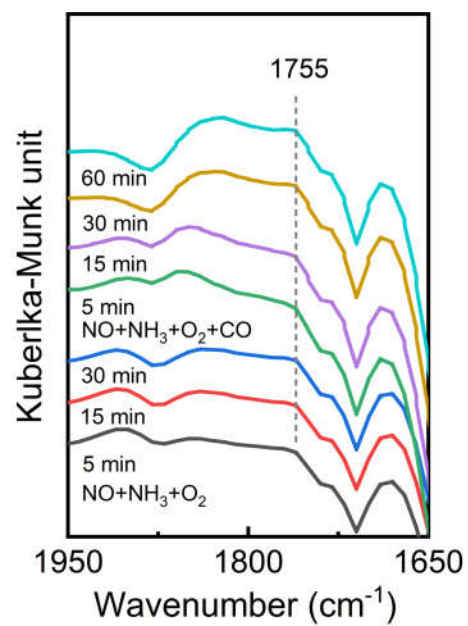
**Fig. S16** NH<sub>3</sub> desorption curves of (a) Cu-SSZ-13 by NH<sub>3</sub> + O<sub>2</sub>-TPD-FTIR experiment and (b) CuO/Cu-SSZ-13 by CO + NH<sub>3</sub> + O<sub>2</sub>-TPD-FTIR experiment.



**Fig. S17** NO desorption curves of (a) Cu-SSZ-13 by NO + O<sub>2</sub>-TPD-FTIR experiment and (b) CuO/Cu-SSZ-13 by CO + NO + O<sub>2</sub>-TPD-FTIR experiment.



**Fig. S18** The  $\text{NH}_3 + \text{NO} + \text{O}_2 + \text{CO}$ -*in situ* DRIFTS spectra of CuO/Cu-SSZ-13 in the range of 3600-3000  $\text{cm}^{-1}$ .



**Fig. S19** The NH<sub>3</sub> + NO + O<sub>2</sub> + CO-*in situ* DRIFTS spectra of CuO/Cu-SSZ-13 in the range of 1950-1650 cm<sup>-1</sup>.

**Table S1** EXAFS fitting parameters at the Cu *K*-edge for CuO/Cu-SSZ-13 and self-prepared CuO.

| Sample        | Shell | $CN^a$        | $R$ (Å) <sup>b</sup> | $\sigma^2$ (Å <sup>2</sup> ) <sup>c</sup> | $\Delta E_0$ (eV) <sup>d</sup> | $R$ factor |
|---------------|-------|---------------|----------------------|-------------------------------------------|--------------------------------|------------|
| CuO           | Cu–O  | $3.6 \pm 0.4$ | $1.91 \pm 0.01$      | $0.0036 \pm 0.0014$                       | $-3.4 \pm 0.6$                 | 0.0035     |
| CuO/Cu-SSZ-13 | Cu–O  | $3.2 \pm 0.4$ | $1.98 \pm 0.01$      | $0.0024 \pm 0.0016$                       | $-0.4 \pm 0.7$                 | 0.0060     |

Notes: <sup>a</sup>coordination number, <sup>b</sup>distance between absorber and backscatter atoms, <sup>c</sup>Debye-Waller factor to account for both thermal and structural disorders, <sup>d</sup>inner potential correction.

**Table S2** Comparison of  $T_{90}$  (CO and NO<sub>x</sub> conversions  $\geq 90\%$ ) and N<sub>2</sub> selectivity  $\geq 90\%$  temperature range with reported literature.

| Catalyst                                                             | Reaction condition                                                                                                                                                                   | Temperature (°C) for NO <sub>x</sub> /CO<br>cov. $\geq 90\%$ and N <sub>2</sub> sel. $\geq 90\%$ | References |
|----------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------|------------|
| CuCeZrO <sub>x</sub> -P                                              | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 9 vol%,<br>[CO] = $1000 \times 10^{-6}$ , GHSV = $40000 \text{ h}^{-1}$                         | 200–360                                                                                          | 1          |
| Pd-V <sub>2</sub> O <sub>5</sub> -MnO <sub>3</sub> /TiO <sub>2</sub> | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $2000 \times 10^{-6}$ , GHSV = $30000 \text{ h}^{-1}$                         | 240–360                                                                                          | 2          |
| CuSmOTi                                                              | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $1000 \times 10^{-6}$ , GHSV = $60000 \text{ h}^{-1}$                         | 175–275                                                                                          | 3          |
| CuMgFeO                                                              | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $600 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $1200 \times 10^{-6}$ , GHSV = $60000 \text{ mL g}^{-1} \text{ h}^{-1}$       | 200–300                                                                                          | 4          |
| CuMnO <sub>x</sub>                                                   | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $600 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $1000 \times 10^{-6}$ , GHSV = $30000 \text{ h}^{-1}$                         | 200–250                                                                                          | 5          |
| Pd/CeNbTiO <sub>x</sub>                                              | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $2000 \times 10^{-6}$ , GHSV = $30000 \text{ h}^{-1}$                         | 240–320                                                                                          | 6          |
| Sm/MnO <sub>x</sub>                                                  | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 11 vol%,<br>[CO] = $1000 \times 10^{-6}$ , GHSV = $60000 \text{ h}^{-1}$                        | 200–275                                                                                          | 7          |
| Ta-CeO <sub>2</sub> /SnO <sub>2</sub>                                | [NO <sub>x</sub> ] = $500 \times 10^{-6}$ , [NH <sub>3</sub> ] = $520 \times 10^{-6}$ , [O <sub>2</sub> ] = 10<br>vol%, [CO] = $5000 \times 10^{-6}$ , GHSV = $25000 \text{ h}^{-1}$ | 325–450                                                                                          | 8          |
| 30Cu/Ce <sub>0.3</sub> Ti <sub>0.7</sub>                             | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $2000 \times 10^{-6}$ , GHSV = $40000 \text{ h}^{-1}$                         | 148–218                                                                                          | 9          |
| CuO/V <sub>2</sub> O <sub>5</sub> -WO <sub>3</sub> /TiO <sub>2</sub> | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $2000 \times 10^{-6}$ , GHSV = $40000 \text{ h}^{-1}$                         | 220–275                                                                                          | 10         |
| CuO/Cu-SSZ-13                                                        | [NO <sub>x</sub> ] = [NH <sub>3</sub> ] = $500 \times 10^{-6}$ , [O <sub>2</sub> ] = 5 vol%,<br>[CO] = $3000 \times 10^{-6}$ , GHSV = $60000 \text{ h}^{-1}$                         | 200–425                                                                                          | This work  |

## References

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