

Supplementary Material for

**Structure-activity relationships, product species distribution and the mechanism of effect of
multi-component flue gas on Hg⁰ adsorption and oxidation over the CuO/AC**

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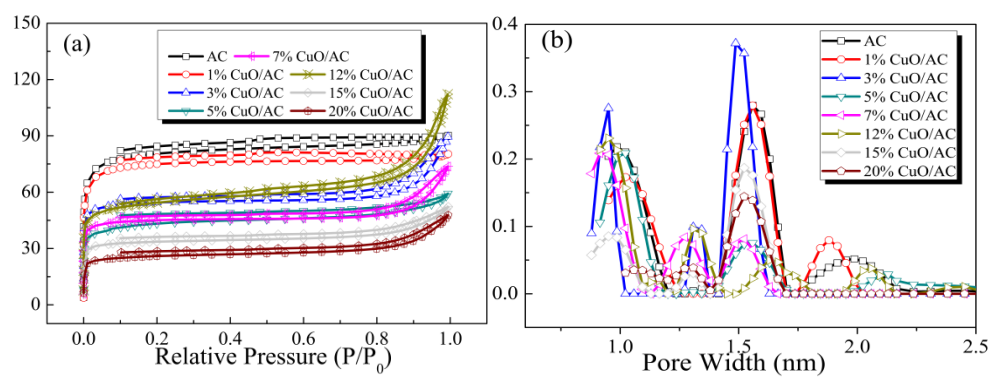


Fig. S1. (a) N₂ adsorption-desorption isotherms and (b) pore size distribution of the catalysts with different CuO contents.

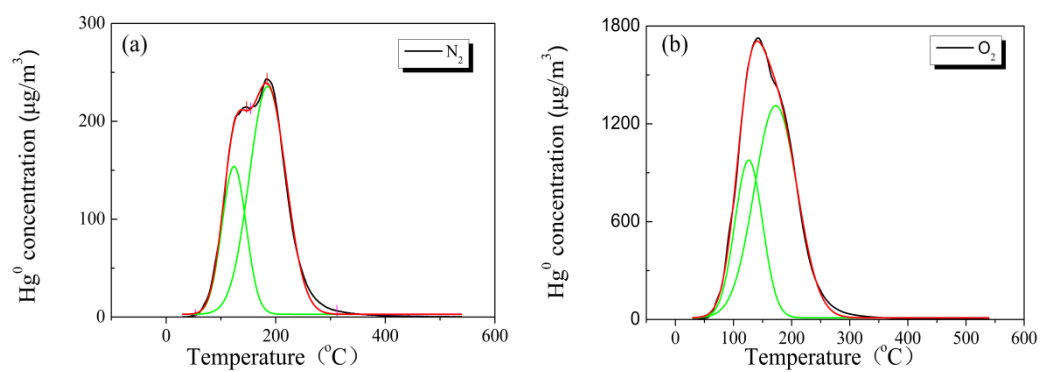


Fig. S2. Deconvoluted Hg^0 -TPD patterns of 12% CuO/AC catalysts after pre-adsorption in N_2 or O_2 atmosphere (a) without N_2 purge and (b) with N_2 purge at 120 $^{\circ}\text{C}$.

Table S1 Hg⁰ removal performance over the different materials.

Materials	Flue gas composition	Hg ⁰ inlet concentration (µg /m ³)	Flow Rate (mL/min)	Temperature (°C)	Removal efficiency (%)	References
Cu-MOFs	N ₂	50	1000	120	91.8	Zhang et al. (2021)
CuO/g-C ₃ N ₄	N ₂	50	1200	120	>98.0	Liu et al. (2018)
CuO/AC-H	N ₂ +5%O ₂	50	300	120	Approximately 70	Zhao et al. (2016)
CoCe/AC	N ₂	105	1000	170	51.6	Wu et al. (2015)
	N ₂ +6%O ₂	105	1000	170	Approximately 80	
Mn-Ce/Ti	N ₂	75	1000	200	40.0	Li et al. (2012)
	N ₂ +10 ppm HCl	75	1000	200	98.0	
	N ₂ +400 ppm SO ₂	75	1000	200	2.1	
	N ₂ +300 ppm NO	75	1000	200	26.7	
V ₂ O ₅ /ZrO ₂ -CeO ₂	N ₂	70	500	250	68.1	Zhao et al. (2016)
	N ₂ +350 ppm NO	70	500	250	79.3	
Materials	Flue gas composition	Hg ⁰ inlet concentration (µg /m ³)	Flow Rate (mL/min)	Temperature (°C)	Breakthrough ratio (%)	References
KI-AC	N ₂	145	600	120	0.72	Tong et al. (2017)
	N ₂ +900 ppm SO ₂	145	600	120	0.40	

Table S2 The average crystallite sizes at the (-110) crystal planes of CuO/AC with different CuO contents.

Samples	Crystallite size (nm)
3% CuO/AC	8
5% CuO/AC	11
7% CuO/AC	11
12% CuO/AC	12
15% CuO/AC	13
20% CuO/AC	13