Supporting Information

Atomically dispersed Au catalysts supported on CeO₂ foam: controllable synthesis and CO oxidation reaction mechanism

Hao Wang, ^a Jianhua Shen, ^a Jianfei Huang, ^b Tengjing Xu, ^a Jingrun Zhu, ^a Yihua Zhu ^{a,*} and Chunzhong Li ^{a,*}

^{a.} Key Laboratory for Ultrafine Materials of Ministry of Education, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai 200237, P. R. China

^{b.} Department of Chemistry and Biochemistry, University of California, Santa Barbara, Santa Barbara 93106, California, United States

*Corresponding author. E-mail: yhzhu@ecust.edu.cn (Prof. Y. H. Zhu) and czli@ecust.edu.cn (Prof. C. Z. Li).



Fig. S1 The schematic of preparing CeO_2 foam in this work.



Fig. S2 TG–DSC curve of the xerogels in this work.



Fig. S3 Nitrogen adsorption/desorption isotherm (A) and the corresponding pore size distribution (B) of the CeO₂ foams.



Fig. S4 Mercury injection test (A) and the corresponding pore size distribution (B) of the CeO₂ foams.



Fig. S5 Rietveld analysis of XRD pattern: experimental data (cycle), final Rietveld refinement (blue line), Bragg positions (vertical line) and difference between both (black line)



Fig. S6 TEM images of Au/F-CeO₂ catalysts with different Au loading amounts: 0.12 wt % (A), 0.54 wt % (B), 1.1 wt % (C), 1.8 wt % (D) and 2.6 wt % (E); HRTEM image and HAADF-STEM images of the 0.12 wt % Au/F-CeO₂ catalyst (F-H).



Fig. S7 The N_2 adsorption-desorption isotherms and corresponding pore size distribution of Au/F-CeO₂ catalysts with different Au loading amounts: 0.12 wt % (A, B), 0.54 wt % (C, D), 1.1 wt % (E, F), 1.8 wt % (G, H) and 2.6 wt % (I, J).



Fig. S8 The detail Au 4f XPS spectrum of 0.12%Au/F-CeO₂ after calcination (A). The Au 4f XPS spectra of Au/F-CeO₂ catalysts before and after calcination with different Au loading amounts: 0.12 wt% (B), 1.1 wt% (C) and 2.6 wt% (D).



Fig. S9 Long-term catalytic stability of 1.1%Au/F-CeO₂ catalyst at 30 °C (A) and corresponding XRD analysis before (a) and after (b) reaction (B).



Fig. S10 Long-term catalytic stability of 0.12%Au/F-CeO₂ catalyst under moisture condition at 80 °C (A) and repeating ignition-extinction cycles of CO conversion under moisture condition at different temperature (B).

Sample	Ce			Au			
	Ce ³⁺ (%)	Ce ⁴⁺ (%)	Lattice O(%)	Adsorbed O(%)	Auº(%)	Au ⁺ (%)	Au ³⁺ (%)
CeO ₂	35.38	64.62	56.46	43.54	*	*	*
0.12%Au/F-CeO ₂	34.45	65.55	76.15	23.85	11.83	65.47	22.70
0.54%Au/F-CeO ₂	32.55	67.45	81.69	18.31	26.82	51.18	21.00
1.1%Au/F-CeO ₂	33.22	66.78	76.50	23.50	46.02	34.50	19.48
1.8%Au/F-CeO ₂	33.75	66.25	70.65	29.35	59.05	26.64	14.31
2.6%Au/F-CeO ₂	34.39	65.61	67.43	32.57	67.16	28.19	4.65

Tab. S1 Surface composition of the samples

Tab. S2 The proportion of metallic Au before and after calcination.

Sample	Before calcination	After calcination
0.12%Au/F-CeO ₂	15.01	11.83
1.1%Au/F-CeO ₂	18.44	46.02
2.6%Au/F-CeO2	17.93	67.16

Sample	$Ce^{3+} 3d_{5/2} (eV)$		$Ce^{4+} 3d_{5/2} (eV)$		$Ce^{3+} 3d_{3/2} (eV)$		$Ce^{4+} 3d_{3/2} (eV)$			
	v_0	v	ν	ν"	ν'''	υ_0	ບ່	ບ່	υ"	υ‴
CeO ₂ foam	880.61	884.52	882.14	888.71	897.22	898.24	902.97	900.68	907.30	916.53
0.12%Au/F-CeO ₂	880.38	884.53	882.22	888.75	897.05	898.33	903.16	900.78	907.32	916.65
0.54%Au/F-CeO ₂	880.99	884.38	882.31	888.64	897.00	898.33	902.96	900.81	907.38	916.69
1.1%Au/F-CeO ₂	880.70	884.60	882.28	888.91	897.00	898.34	903.16	900.82	907.39	916.68
1.8%Au/F-CeO ₂	880.70	884.33	882.28	888.70	897.29	898.39	902.83	900.82	907.44	916.70
2.6%Au/F-CeO ₂	880.76	884.43	882.42	888.81	897.29	898.52	902.74	900.94	907.57	916.85

Tab. S3 The assignment of Ce 3d photoelectron peaks of the samples.

 Tab. S4 Specific rates and TOFs of the Au/F-CeO₂ catalysts in this work compared with some typical supported catalysts reported in literature.

Catalysts	Au loading (wt%)	Temperature (°C)	Specific rate (mol _{CO} h ⁻¹ g _{Au} ⁻¹)	TOF (s ⁻¹)	
1.1%Au/F-CeO ₂	1.1	80	2.97	1.1041 ^a	this work
0.12%Au/F-CeO ₂	0.12	80	26.12	1.4294 ^b	this work
2Au/CeO ₂ -DP	2.0	80	10.2	1.9°	ref. 14
1Au/CeO ₂ -RRCe	0.98	80	2.6	0.64°	ref. 14
Au/CeO ₂	3.0	80	≈4.5 ^d	*	ref. 43
Au/CeO ₂	1.0	100	1.6	*	ref. 44
Au/Fe ₂ O ₃ -WGC	4.4	80	0.8	0.17	ref. 45

^{*a*}Calculated with 14.7307% dispersion. ^{*b*}Calculated with 100% dispersion. ^{*c*}Dispersion was calculated based on the relation of $D=1/d_{Au}$. ^{*d*}Calculated by extrapolating the rate at 50 °C based on their activation energy.