Supplementary materials for

Divergent influence of {1 1 1} vs {1 0 0} crystal planes and Yb³⁺ dopant on CO oxidation paths in mixed oxide nano-sized Au/Ce_{1-x}Yb_xO_{2-x/2} (x = 0 or 0.1) systems.

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Fig.S1. TEM images of CeO₂ (octahedron-like) prepared by methods which using (A),(B) NH₄OH, (C),(D) urea, (E),(F) without mineralizer (250 °C).



Fig.S2. TEM images of CeO₂ and Ce_{0.9}Yb_{0.1}O_{1.95} after heat treatment at 200 °C and 400 °C under reducing conditions and 300 °C in static air.



Fig.S3. TEM images of Au/CeO₂ and Au/Ce_{0.9}Yb_{0.1}O_{1.95} after heat treatment at 200 °C and 400 °C under reducing conditions and 300 °C in static air.



Fig.S4. Histograms of the Au nanoparticles sizes calculated for Au/CeO₂ and Au/Ce_{0.9}Yb_{0.1}O_{1.95} after heat treatment at 200 °C and 400 °C under reducing conditions and 300 °C in static air.



Fig.S5. HRTEM image of Au/Ce_{0.9}Yb_{0.1}O_{1.95}C heated at 400 °C for 3h in H₂ flow.

Table 1S

Misfit values between Au and CeO₂ crystals (%misfit = $(d_{Au} - d_{support}) / d_{support}$) x 100)

Misfit in %	Au planes	Misfit in %
For octahedron-like ceria		For cube-like ceria
d 1 1 $1_{CeO2} = 0.3124 \text{ nm}$		d 1 0 $0_{CeO2} = 0.2706 \text{ nm}$
24%	d 1 1 $1_{Au} = 0.2355 \text{ nm}$	13%
35%	$d \ 2 \ 0 \ 0_{Au} = 0.2039 \ nm$	25%
54%	$d 2 2 0_{Au} = 0.1442 \text{ nm}$	47%
61%	$d 3 1 1_{Au} = 0.1230 \text{ nm}$	55%



Fig.S6. The divergent influence of $\{1 \ 1 \ 1\}$ vs $\{1 \ 0 \ 0\}$ crystal planes and Yb3+ dopant on CO oxidation paths in mixed oxide nano-sized Au/Ce1-xYbxO2-x/2 (x = 0 or 0.1; O or C) systems (CO oxidation activity).



Fig.S7. CO oxidation by O_2 on ceria based oxide as a catalyst.



Fig.S8. CO oxidation by O_2 on ceria based oxide decorated by nanocrystalline Au as a catalyst.

Table 2S

The oxygen vacancy (Ov) formation energies of pure and Co-doped ceria 1 1 1 and 1 0 0 facets – literature data [Phys. Chem. Chem. Phys., 20 (2018) 16045-16059]

Sample/facet	CeO ₂	Co-CeO ₂
111	2.42 eV	-0.08 eV
100	1.75 eV	0.24 eV