Supplementary Materials: Effect of an Sb-Doped SnO_2 Support on the CO-Tolerance of Pt_2Ru_3 Nanocatalysts for Residential Fuel Cells

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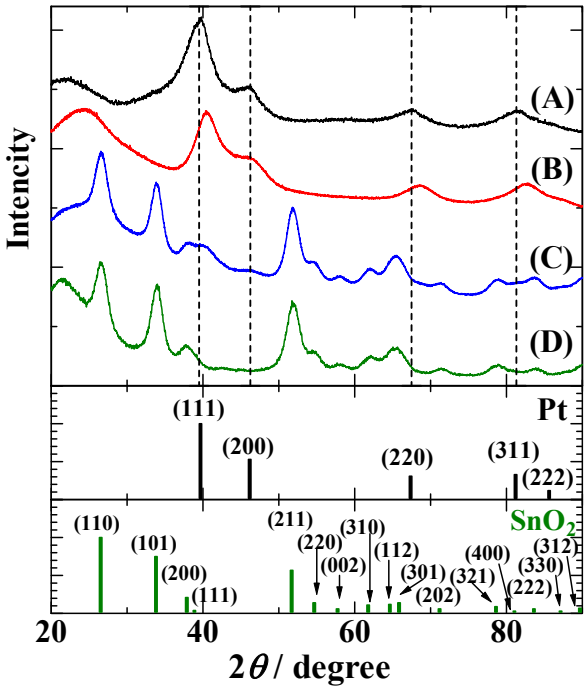

Figure S1. X-ray diffraction patterns of pristine powders of (**A**) commercial Pt/CB (50 wt %-Pt, TEC10E50E); (**B**) Pt_2Ru_3/CB; (**C**) Pt2Ru_3/Sb-SnO_2; and (**D**) Sb-SnO_2 support and the assignment of XRD peaks to Pt and SnO_2. Dashed vertical lines indicate the positions of diffraction peaks for pure platinum.

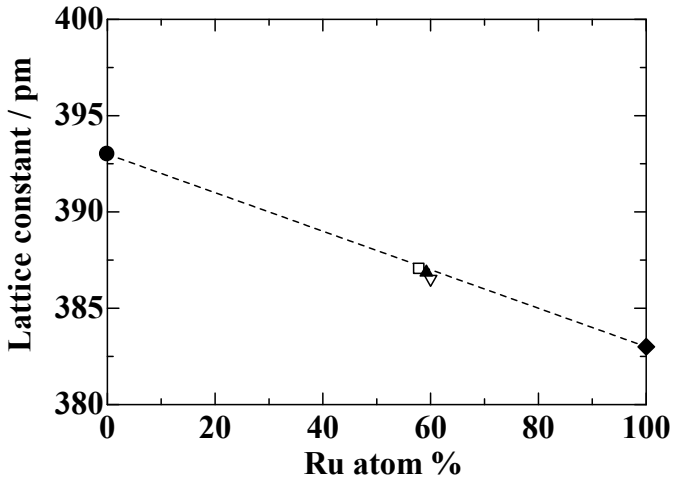

Figure S2. Relationship between lattice constant and Ru content (analyzed atomic percent) of Pt_2Ru_3 alloys for (▲) Pt_2Ru_3/CB, (□) Pt_2Ru_3/Sb-SnO_2, and (▽) commercial Pt_2Ru_3/CB. Symbols (●) and (◆) indicate the lattice constant of pure Pt and Ru, and the dotted line indicates the Vegard's law.

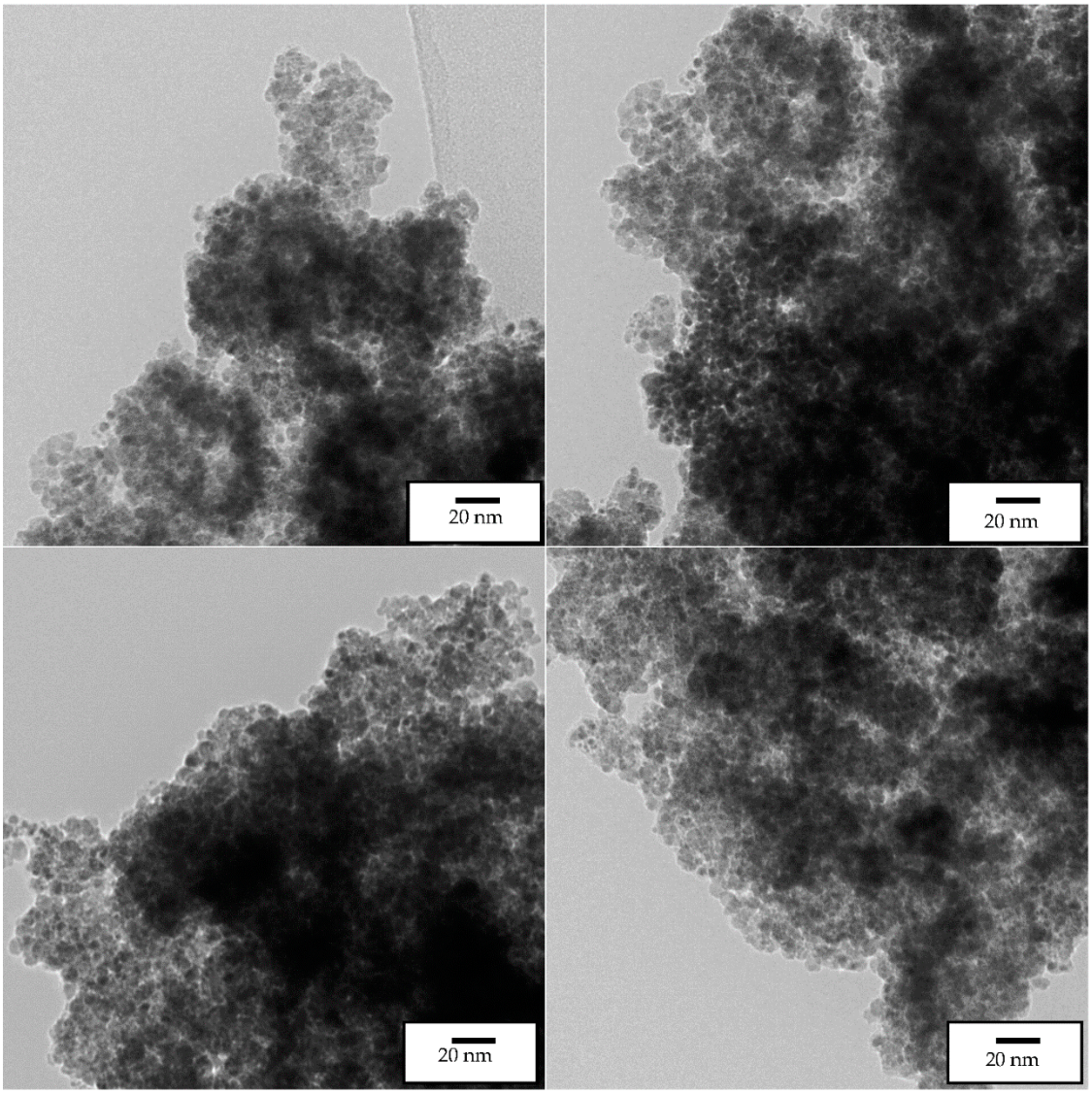

Figure S3. Additional TEM images of pristine Pt_2Ru_3/Sb-SnO_2.

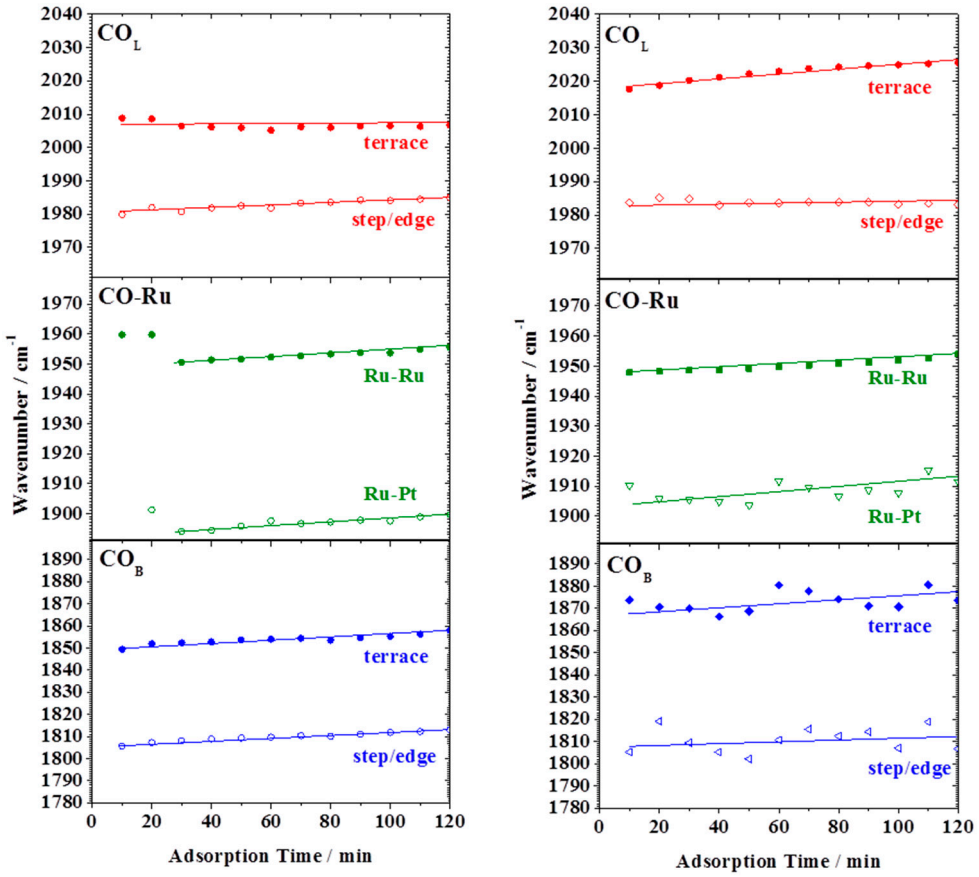

Figure S4. Peak top wavenumbers of CO_L, CO-Ru, and CO_B observed at 0.02 V and 60 °C in 1% CO (H_2-balance)-saturated 0.1 M $HClO_4$.

Table S1. Values of peak wavenumber and the full width at half maximum (FWHM) used for the deconvolution of FTIR spectra on Pt_2Ru_3/CB and Pt_2Ru_3/Sb-SnO_2 shown in Figures 5 and 6. The integrated intensity of each peak after 2 h of CO adsorption is also shown.

Peak Wavenumber (cm^{-1})		FWHM (cm^{-1})	Assignment	Integrated Intensity after 2 h (Abs. cm^{-1})	
Pt_2Ru_3/CB	Pt_2Ru_3/Sb-SnO_2	-	-	Pt_2Ru_3/CB	Pt_2Ru_3/Sb-SnO_2
2006	2025	33	CO_L, Pt terrace	0.186	0.265
1985	1983	36	CO_L, Pt step/edge	0.156	0.134
1955	1953	55	CO_B, Ru-Ru	0.119	0.119
1900	1911	35	CO_B, Ru-Pt	0.017	0.030
1857	1873	45	CO_B, Pt terrace	0.005	0.029
1813	1806	72	CO_B, Pt step/edge	0.010	0.023

Appendix S1. Calculation of the number of atoms at terraces and step/edges of a cubo-octohedral Pt_2Ru_3 fcc particle with the particle size d, according to the method in [25,26].

First, we calculated the number of total atoms N_{total} included in the particle with the number of atom layers m:

$$N_{total} = (10/3)m^3 - 5m^2 + (11/3)m - 1 \quad \text{(S1)}$$

As a measure of the particle size, we calculated d for a sphere having N_{total} atoms:

$$d = a_{PtRu}\,(3N_{total}/2\pi)^{1/3} \quad \text{(S2)}$$

where a_{PtRu} is the lattice constant of the Pt_2Ru_3 alloy.

Next, the number of surface atoms was calculated by the following equation [25]:

$$N_{surface} = 10m^2 - 20m + 12 \quad \text{(S3)}$$

Then, the number of atoms at step/edges $N_{step/edge}$ as well as that at terraces were calculated:

$$N_{step/edge} = 12 \text{ (atoms at vertex)} + 24(m - 2) \quad \text{(S4)}$$

$$N_{terrace} = N_{surface} - N_{step/edge} \quad \text{(S5)}$$

By using an average particle size d = 2.6 nm based on the TEM observation, we obtained these values shown below:

Table S2. Number of atoms calculated based on a cubo-octohedral shape of Pt_2Ru_3 fcc nanoparticles.

***d* (nm)**	**Number of layers, *m***	**Number of Total Surface Atoms, $N_{surface}$**	**Number of Atoms at Step/Edges, $N_{step/edge}$**	**Number of Atoms at Terraces, $N_{terrace}$**
2.6	6	252	108	144