Supporting Information

On the Role of Ce towards CO_2 Adsorption and Activation over Lanthanum Species

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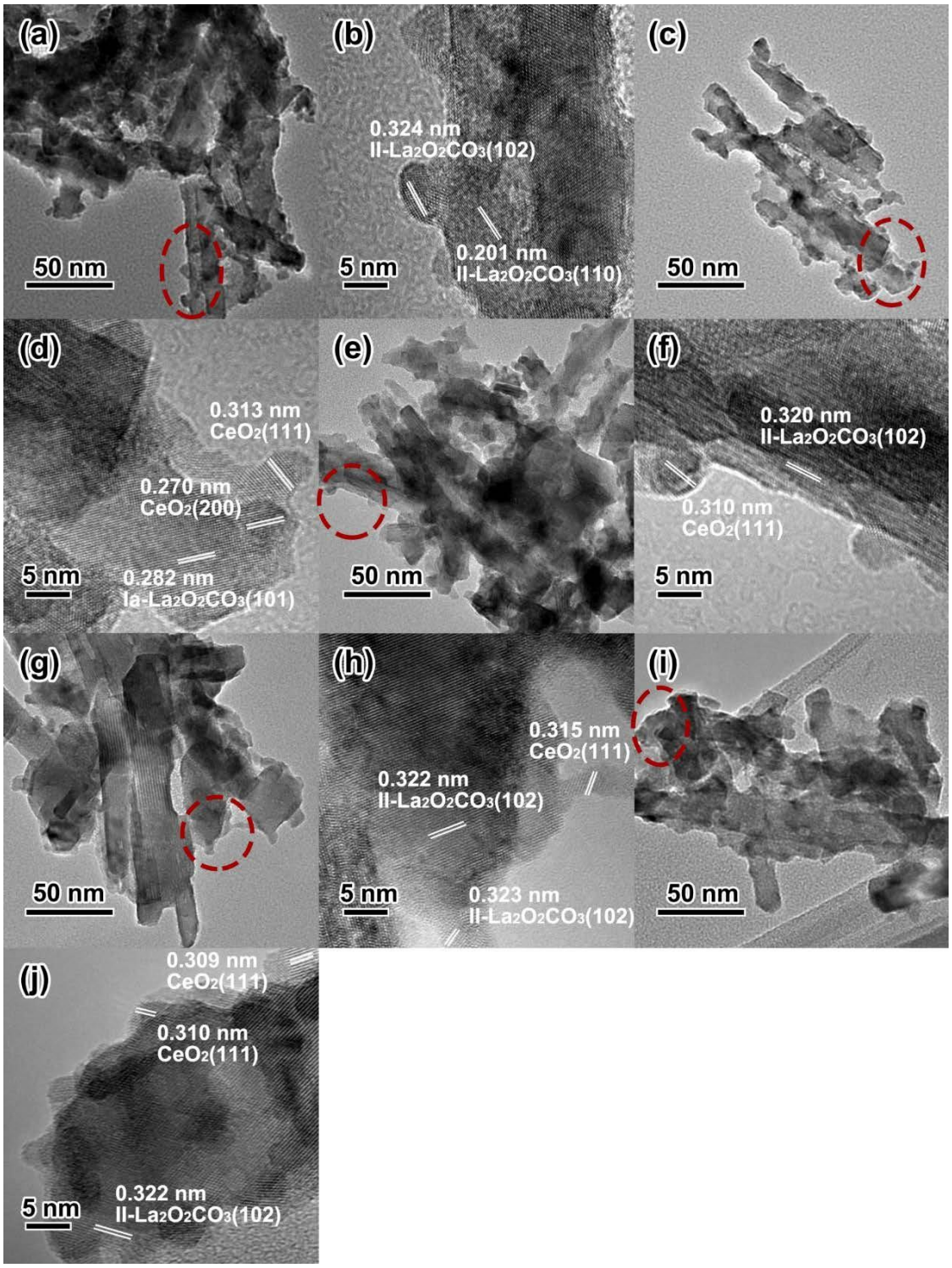

Figure S1. HR-TEM images of the series of Ce-La mixed oxide after CO_2 adsorption for 30 min. (a, b) $La_2O_2CO_3$, (c, d) 0.05Ce-LOC, (e, f) 0.10Ce-LOC, (g, h) 0.15Ce-LOC, (i, j) 0.20Ce-LOC.

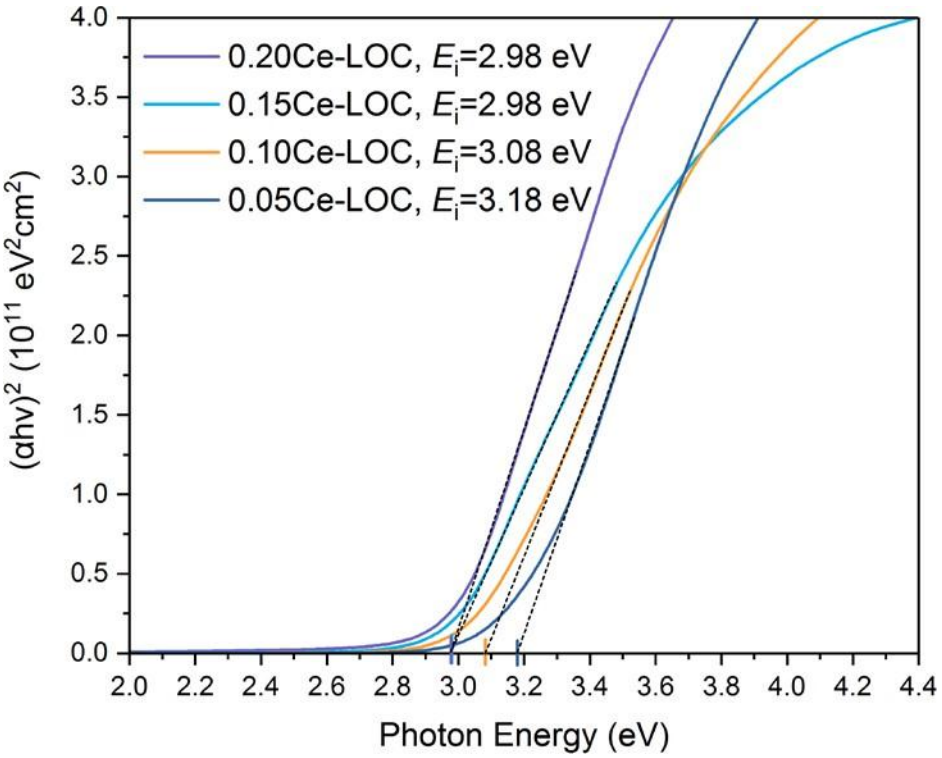

Figure S2. Plots of $(ahv)^2$ vs photon energy for the series of Ce-La mixed oxides.

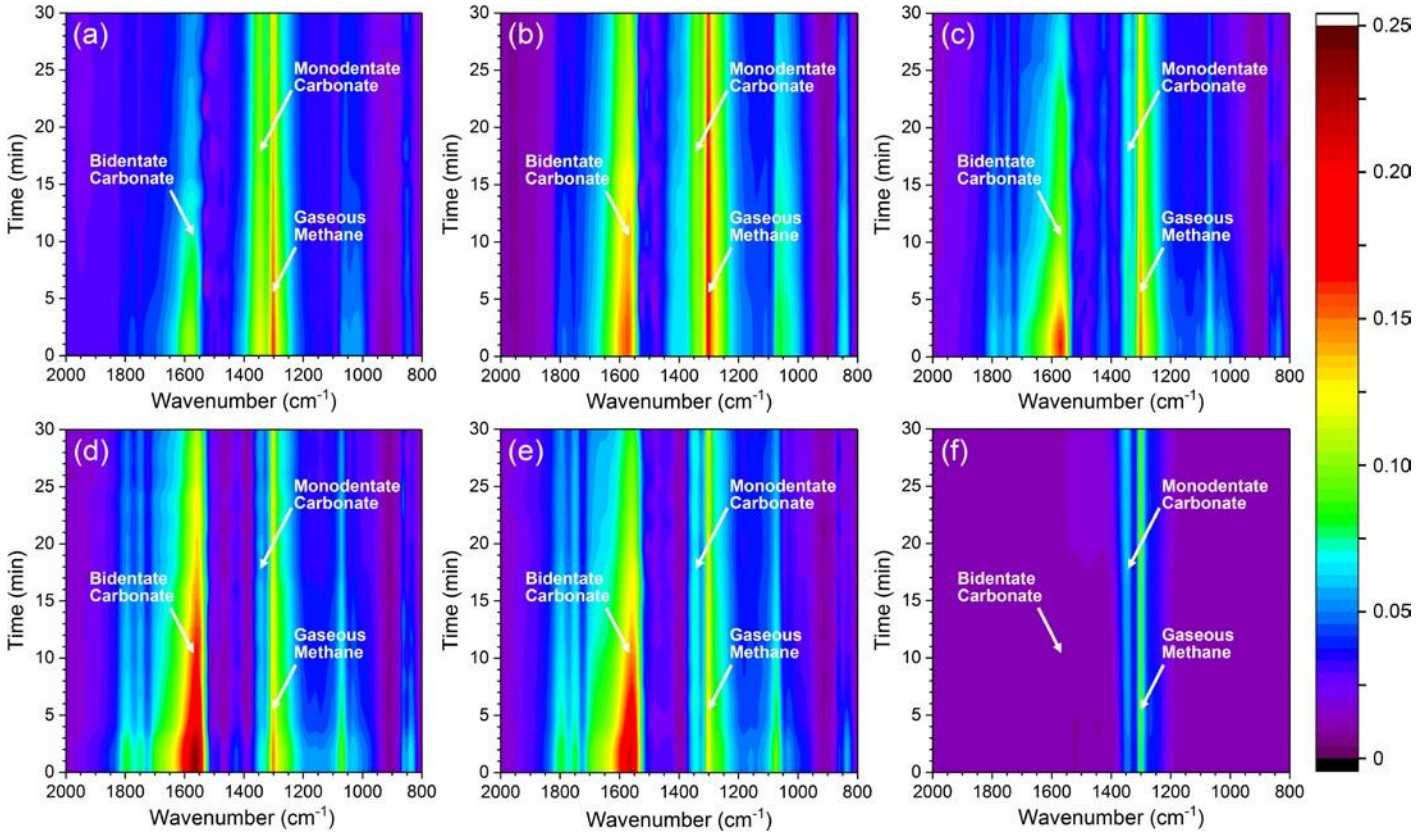

Figure S3. Contour graphs of DRIFTS spectra for the series of Ce-La mixed oxide during CH_4 adsorption for 30 min. (a) 0Ce-LOC, (b) 0.05Ce-LOC, (c) 0.10Ce-LOC, (d) 0.15Ce-LOC, (e) 0.20Ce-LOC and (f) CeO_2.

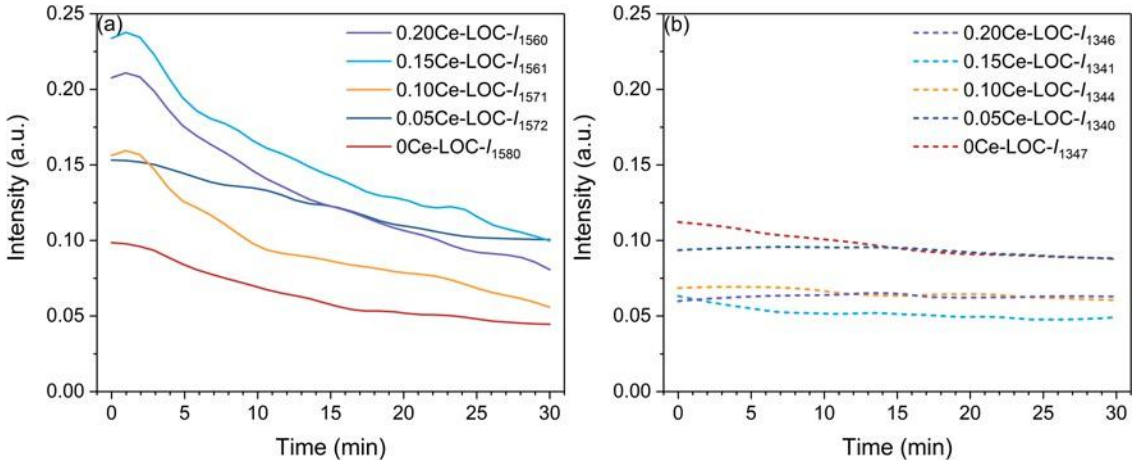

Figure S4. The intensity of peaks in DRIFTS spectra as a function of time on stream. (a) Bidentate carbonate, (b) Monodentate carbonate.

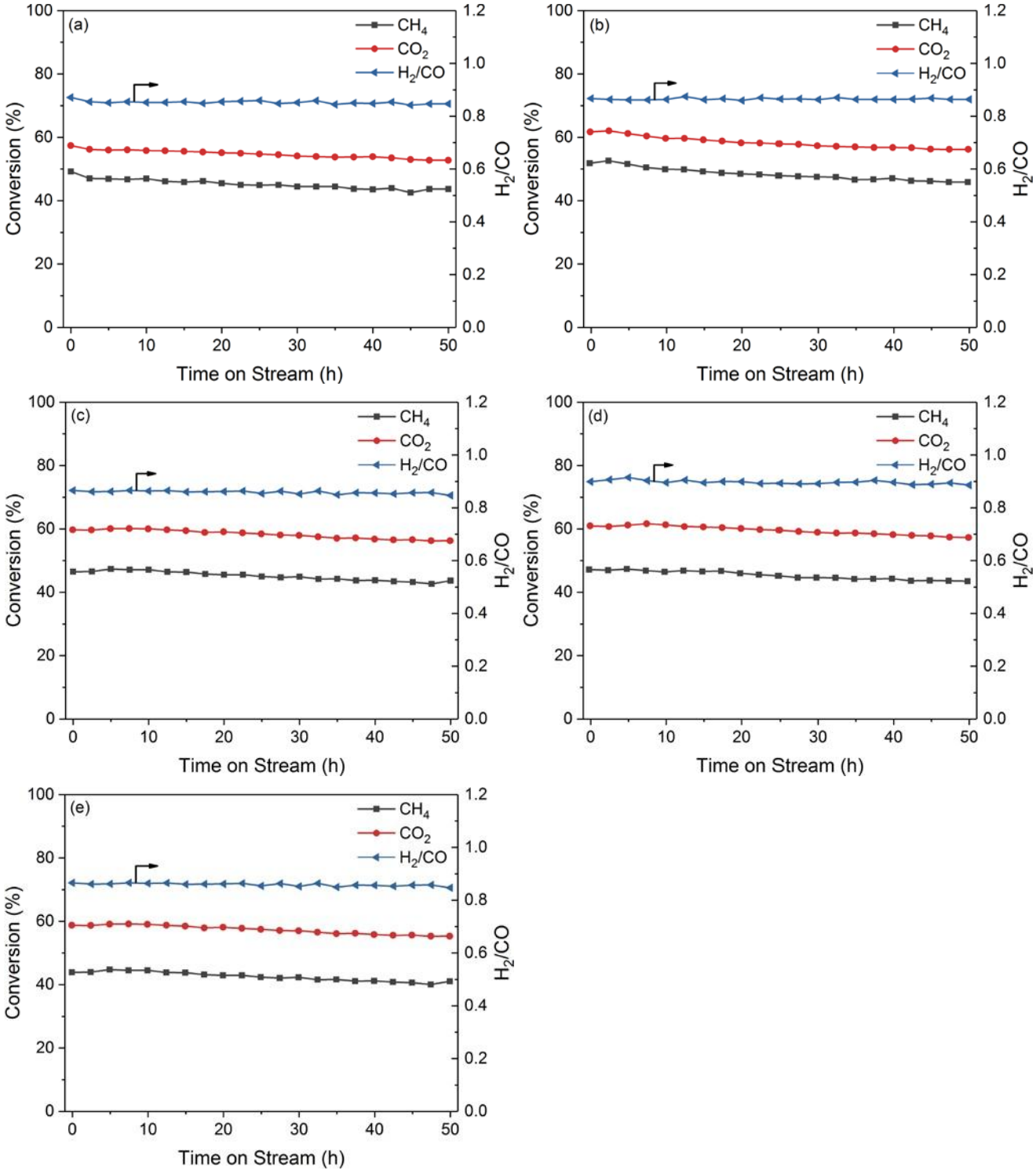

Figure S5. Activity test of the catalysts. CH_4 and CO_2 conversions as a function of time on stream over the catalysts including relevant H_2/CO ratio. (a) 5Ni/0Ce-LOC, (b) 5Ni/0.05Ce-LOC, (c) 5Ni/0.10Ce-LOC, (d) 5Ni/0.15Ce-LOC, and (e) 5Ni/0.20Ce-LOC.Reaction conditions: $CH_4/CO_2/N_2 = 20/20/60$, GHSV = 60,000 $mL \cdot h^{-1} \cdot g_{cat}^{-1}$, 650 °C, 1 atm.

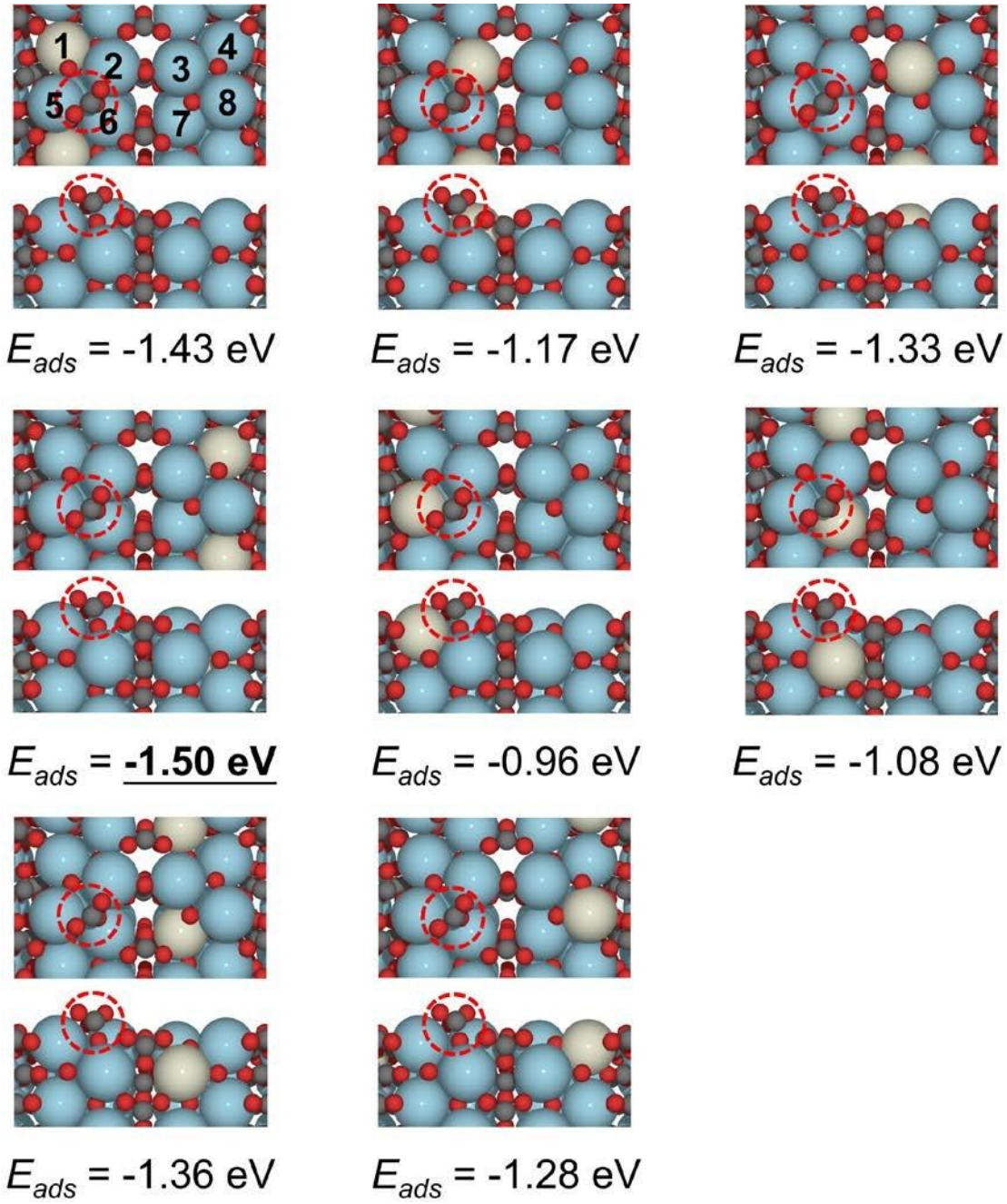

Figure S6. Possible models for 1Ce-doping and corresponding calculated CO_2 adsorption energies.

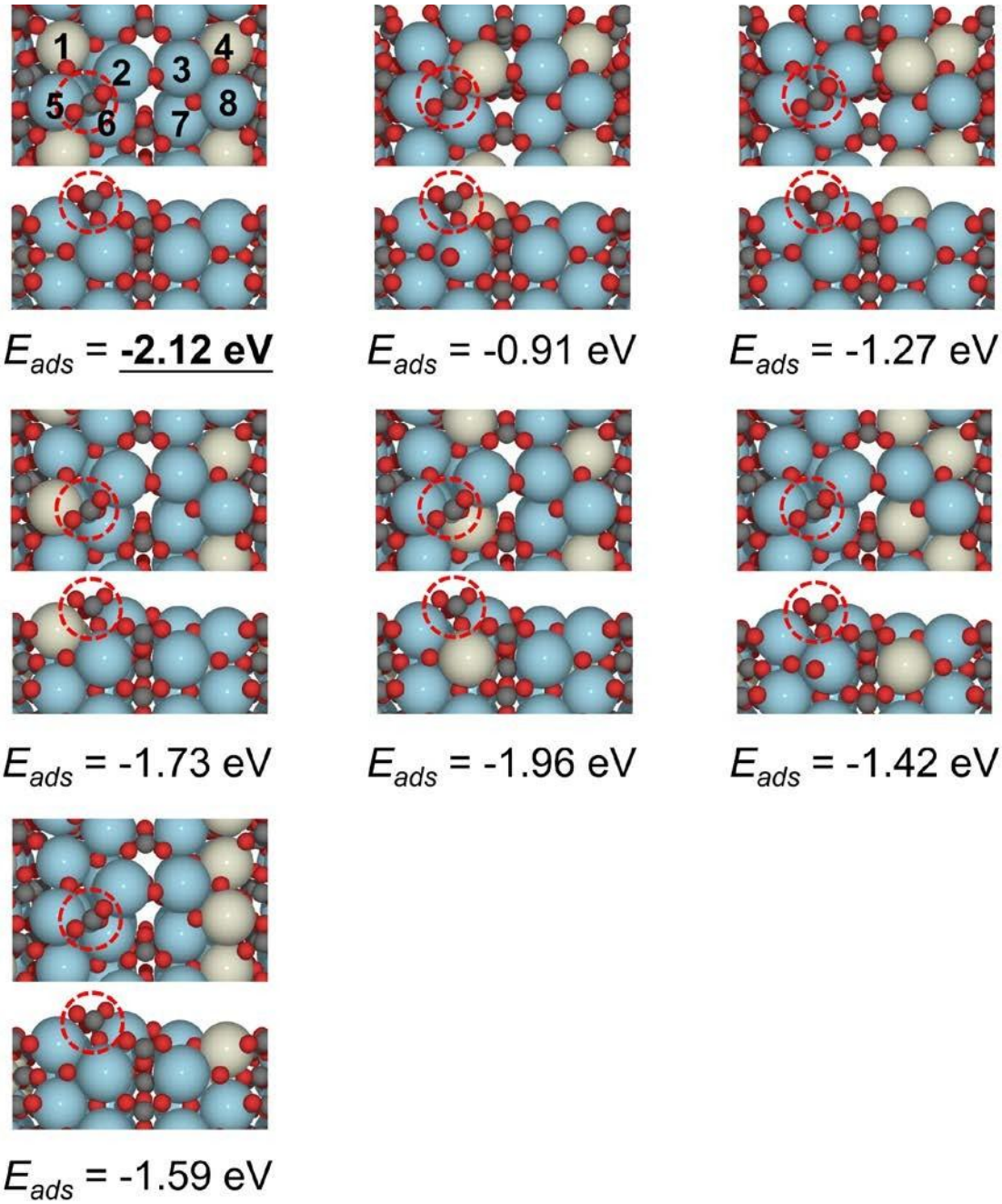

Figure S7. Possible models for 2Ce-doping and corresponding calculated CO_2 adsorption energies.

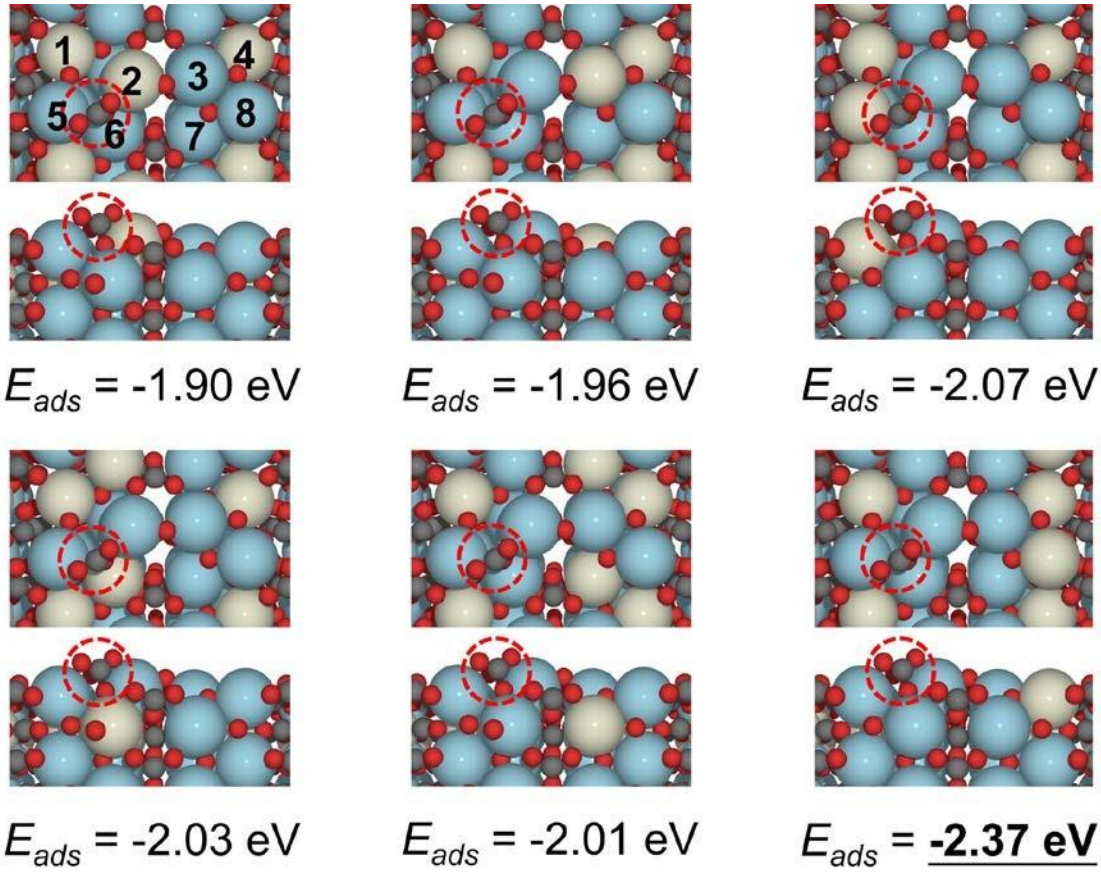

Figure S8. Possible models for 3Ce-doping and corresponding calculated CO_2 adsorption energies.

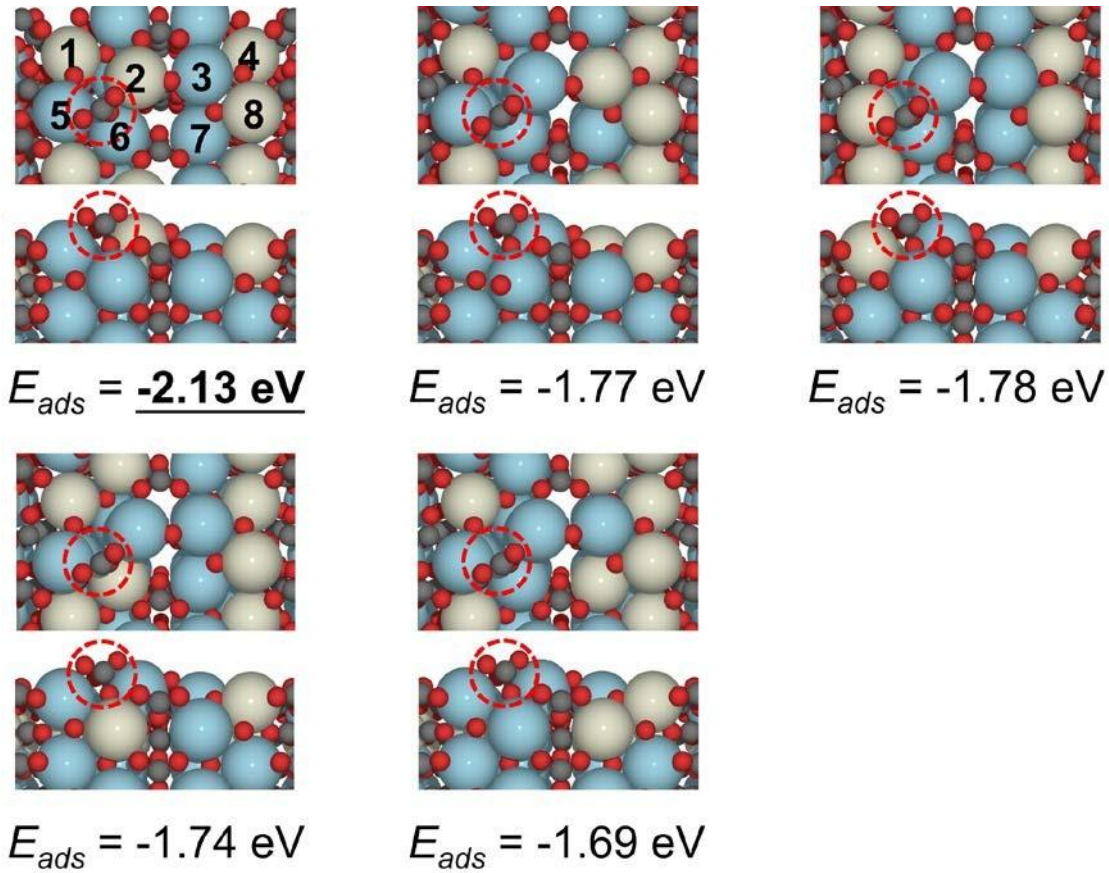

Figure S9. Possible models for 4Ce-doping and corresponding calculated CO_2 adsorption energies.

Table S1. Calculated CO_2 adsorption energies with randomly distributed Ce structures.

2Ce-doping		3Ce-doping		4Ce-doping	
Ce position[a]	E_{ads} / eV	Ce position	E_{ads} / eV	Ce position	E_{ads} / eV
3 and 8	-1.29	4, 6 and 7	-1.66	3, 4, 7, and 8	-1.28
3 and 5	-1.66	1, 4 and 7	-2.05	2, 3, 5, and 8	-1.78
5 and 8	-1.60	1, 3 and 5	-2.36	1, 3, 5, and 7	-1.74
6 and 7	-1.62			1, 2, 3, and 6	-1.69
1 and 7	-2.06			2, 4, 5, and 7	-1.31
7 and 8	-1.35			1, 2, 4, and 5	-1.92
1 and 5	-1.55			1, 2, 5, and 6	-1.36
5 and 6	-1.63			1, 3, 4, and 5	-2.04
2 and 3	-1.16				

[a] See definition in Figure 11.