Supporting Information

for

CO oxidation mechanism on CeO_2 supported Au nanoparticles

Hyun You Kim*, Hyuck Mo Lee, and Graeme Henkelman

Micro kinetic model for CO oxidation by coadsorbed CO and O_2 on Au_{13}@CeO_2-STO and Au_{13}@CeO_2-3VAC

The micro-kinetic model for CO oxidation by coadsorbed CO and O_2 on Au_{13}@CeO_2-STO and Au_{13}@CeO_2-3VAC which presented in Figure 7 and Figure S3 is simply as follows:

$CO(g) + * \Leftrightarrow CO*$ (R1)

$O_2(g) + * \Leftrightarrow O_2*$ (R2)

$CO* + O_2* \Leftrightarrow CO_2(g) + O* + *$ (R3)

$CO* + O* \Leftrightarrow CO_2(g) + 2*$ (R4)

Here, the rate of CO_2 formation is equal to the maximum of the rate of the reaction R3. Because the first two reactions are in equilibrium, the rate of these reactions can be written as follows:

$$\text{rate(R1)} = k_1^+ p(CO)\theta_* - k_1^- \theta_{CO} \;\rightarrow\; \theta_{CO} = \left({}^{k_1^+}\!/_{k_1^-} \right) p(CO)\theta_* = K_1 P(CO)\theta_*$$

$$\text{rate(R2)} = k_2^+ p(O_2)\theta_* - k_2^- \theta_{O_2} \;\rightarrow\; \theta_{O_2} = \left({}^{k_2^+}\!/_{k_2^-} \right) p(O_2)\theta_* = K_2 P(O_2)\theta_*$$

The rate of CO_2 formation, rate(R3)^{max} is as follows:

$$\text{rate(R3)}^{max} = k_3^+ \theta_{CO}\theta_{O_2} = k_3^+ K_1 K_2 p(CO) p(O_2) {\theta_*}^2$$

where K_1 and K_2 are the equilibrium constants for R1 and R2, p(CO) and $p(O_2)$ are the partial pressures of CO and O_2. k_i^+ and k_i^- represents the forward and the backward reaction constant for Ri, respectively.

Because the sum of the coverage of adsorbed O_2, CO and free adsorption sites should be equal to 1, we can numerically derive θ_* from θ_{CO} and θ_{O_2}:

$$\theta_{CO} + \theta_{O_2} + \theta_* = 1 \;\rightarrow\; \theta_* = \frac{1}{1 + K_1 p(CO) + K_2 p(O_2)}$$

where θ_{CO}, θ_{O_2}, and θ_* are the coverage of adsorbed CO, adsorbed O_2, and free sites of the surface. Because R4 is very fast, θ_O is negligibly small. It was set to zero.

Note that the reaction R1 and R2 concerns the adsorption of CO and O_2,

respectively.

Therefore, the rate constants K1 and K2 are,

$$K1 = \exp\left(\frac{-\Delta G1}{kT}\right) = \exp\left(\frac{-(\Delta E1 - T\Delta S1)}{kT}\right)$$

$\Delta E1$: Energy of CO adsorption

$\Delta S1$: Entropy change involved in CO adsorption

and

$$K2 = \exp\left(\frac{-\Delta G2}{kT}\right) = \exp\left(\frac{-(\Delta E2 - T\Delta S2)}{kT}\right)$$

$\Delta E2$: Energy of O_2 adsorption

$\Delta S2$: Entropy change involved in O_2 adsorption

For R3, the maximum rate can be obtained as follows:

$$\text{rate}(R3)^{max} = k_3^+ \theta_{CO} \theta_{O_2} = k_3^+ K_1 K_2 p(CO) p(O_2) {\theta_*}^2$$

where,

$$k_3^+ = \frac{kT}{h} \exp\left(\frac{-\Delta G3^+}{kT}\right) = \frac{kT}{h} \exp\left(\frac{-(E_{act} - T\Delta S3^+)}{kT}\right)$$

E_{act} : Activation energy for reaction 3

$\Delta S3^+ = 0$

rate(R3)^{max} was calculated for CO oxidation process described in Figure 7 at T=298 K, p(CO)=0.01 bar, p(O_2)=0.21 bar, $\Delta S1 = 205.1\ J/mol \cdot K$, and $\Delta S2$ =197.7 $J/mol \cdot K$. Results are listed in Table 1.

Table S1. Energy of adsorption of Au_{13} on stoichiometric and partially reduced CeO_2 surfaces

	Stoichiometric	Partially reduced CeO_2 (CeO_2-nVAC)[a]		
	CeO_2	CeO_2-1VAC	CeO_2-2VAC	CeO_2-3VAC
Energy of Au_{13} adsorption (eV)	-3.15	-3.35	-3.78	-4.11

[a] n is a number of surface oxygen vacancy in the CeO_2 support

Table S2. Relative stability of negatively and positively charged Au_{13} isomers[a]

Au_{13}^-	Neutral Au_{13}	Au_{13}^+
Cage2	Planar	3D1
Cage1 (0.02)	Cage1 (0.11)	3D2 (0.16)
Planar (0.10)	Cage2 (0.14)	Planar (0.22)
3D2 (0.16)	3D1 (0.21)	Cage1 (0.73)
3D1 (0.89)	3D2 (0.23)	Cage2 (0.80)

[a] Calculated with DMol[3] code. Relative energy to the most stable structure was presented in parenthesis. Refer to Figure 2 for the structure of Au_{13} isomers.

Table S3. Charge dependent stability of Au_{13}-3D2 NPs[a]

Au_{13}-3D2	ΔE (eV)
Au_{13}^{+2}	16.90
Au_{13}^{+1}	6.46
Au_{13}	0
Au_{13}^{-1}	-3.64
Au_{13}^{-2}	-2.76

[a] Refer to Figure 2 for the geometry of Au_{13}-3D2

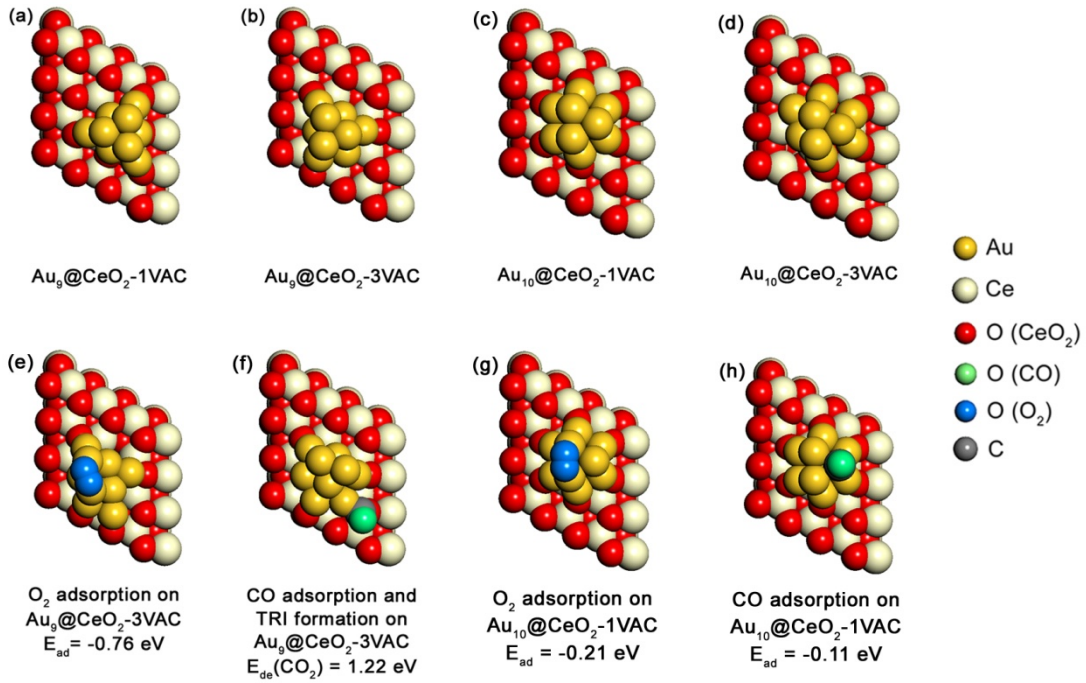

Figure S1. Morphology of fcc-like Au_9 and hcp-like Au_{10} supported on reduced-CeO_2 surfaces: (a) Au_9@CeO_2-1VAC, (b) Au_9@CeO_2-3VAC, (c) Au_{10}@CeO_2-1VAC, and (d) Au_{10}@CeO_2-3VAC. O_2 and CO adsorption on Au_9@CeO_2-3VAC and Au_{10}@CeO_2-1VAC: (e) O_2 on Au_9@CeO_2-3VAC, (f) CO on Au_9@CeO_2-3VAC (TRI formation), (g) O_2 on Au_{10}@CeO_2-1VAC, and (h) CO on Au_{10}@CeO_2-1VAC. Au_9 was stable on both CeO_2-1VAC and CeO_2-3VAC but adsorption induced structural disorder occurs at Au_9@CeO_2-3VAC. Although Au_{10} was stable on CeO_2-1VAC, more vacancies in the CeO_2 surface leads to the highly distorted Au_{10}.

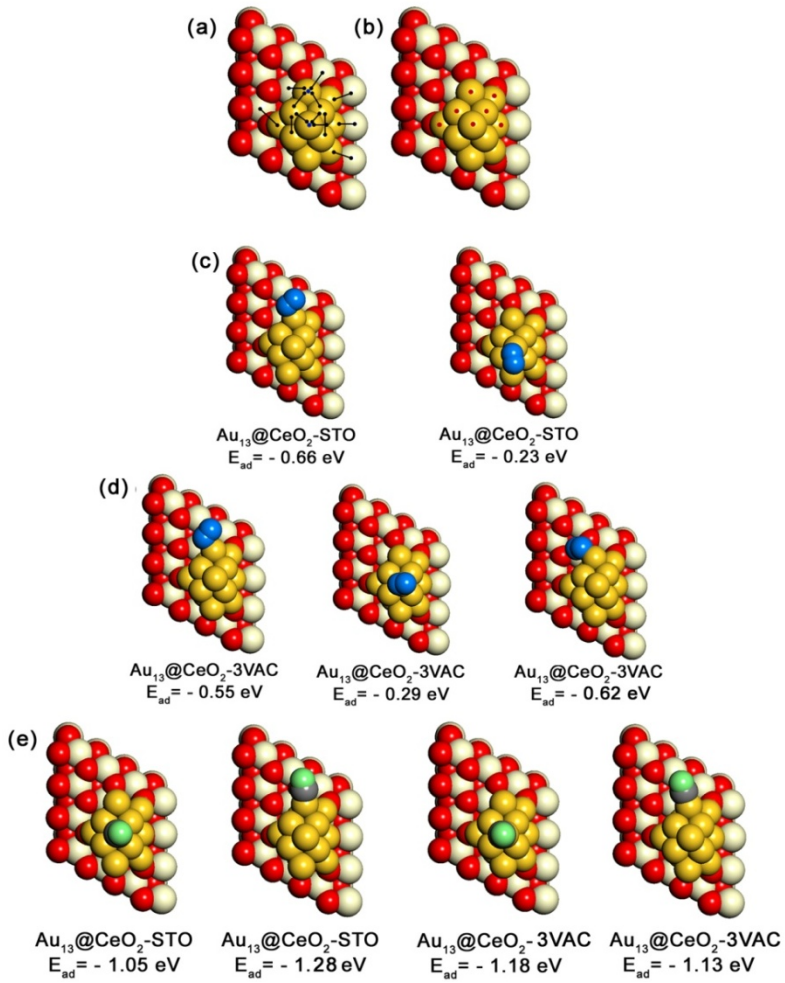

Figure S2. CO and O_2 adsorption on $Au_{13}@CeO_2$-STO and $Au_{13}@CeO_2$-3VAC. (a) and (b) shows where the O_2 and CO adsorption was tested, respectively. Black rods and blue dots in (a) represent the two-site parallel bonding or the single-site perpendicular bonding positions. Red dots in (b) denotes where the CO binding was calculated. (c) and (d) shows the most favorable O_2 binding sites of $Au_{13}@CeO_2$-STO and $Au_{13}@CeO_2$-3VAC, respectively. (e) shows the two strong CO binding sites on $Au_{13}@CeO_2$-STO and $Au_{13}@CeO_2$-3VAC.

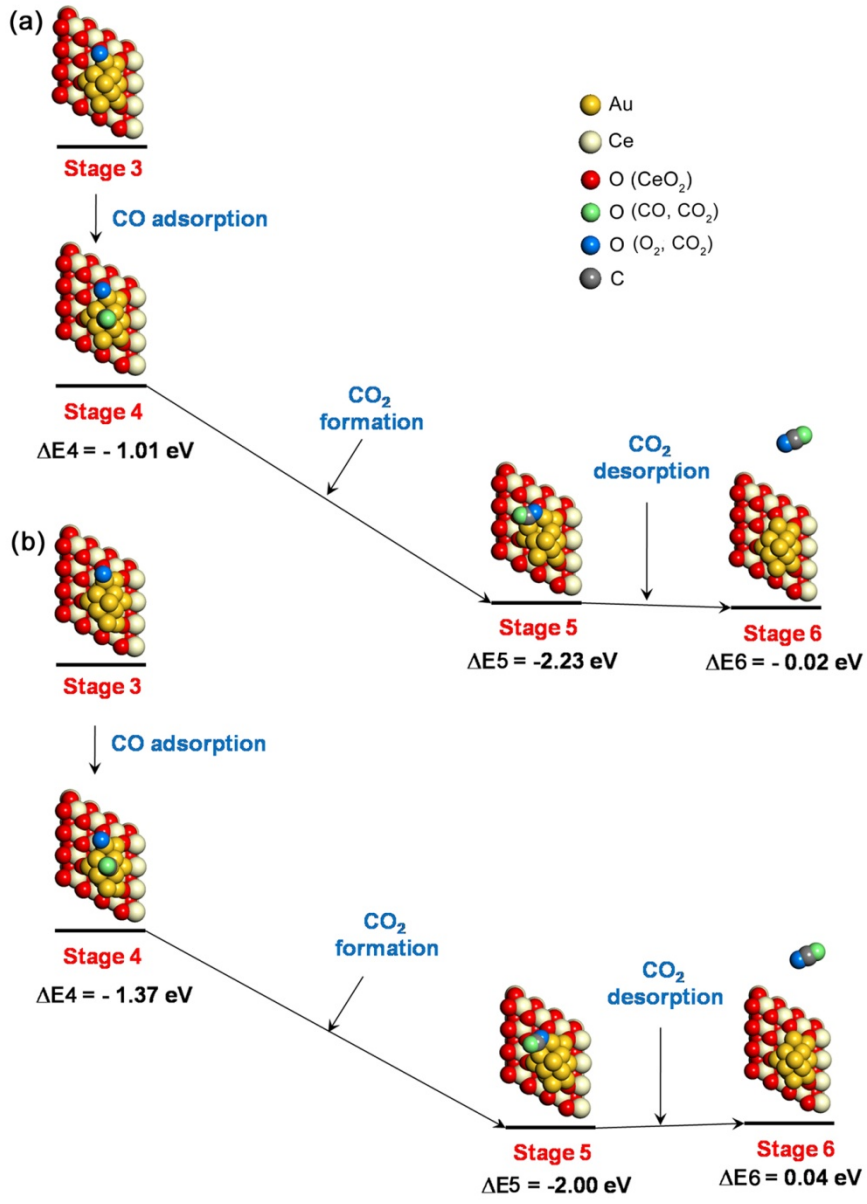

Figure S3. The spontaneous CO oxidation by the residual Au-O^* is shown through the association of Au-O^* and Au-CO^* and subsequent CO_2 formation. Au_{13}@CeO_2-STO is shown in (a) and Au_{13}@CeO_2-3VAC in (b). Direct CO oxidation from stage 4 to stage 6 occurs. CO^*+O^* coupling is barrierless in both cases.

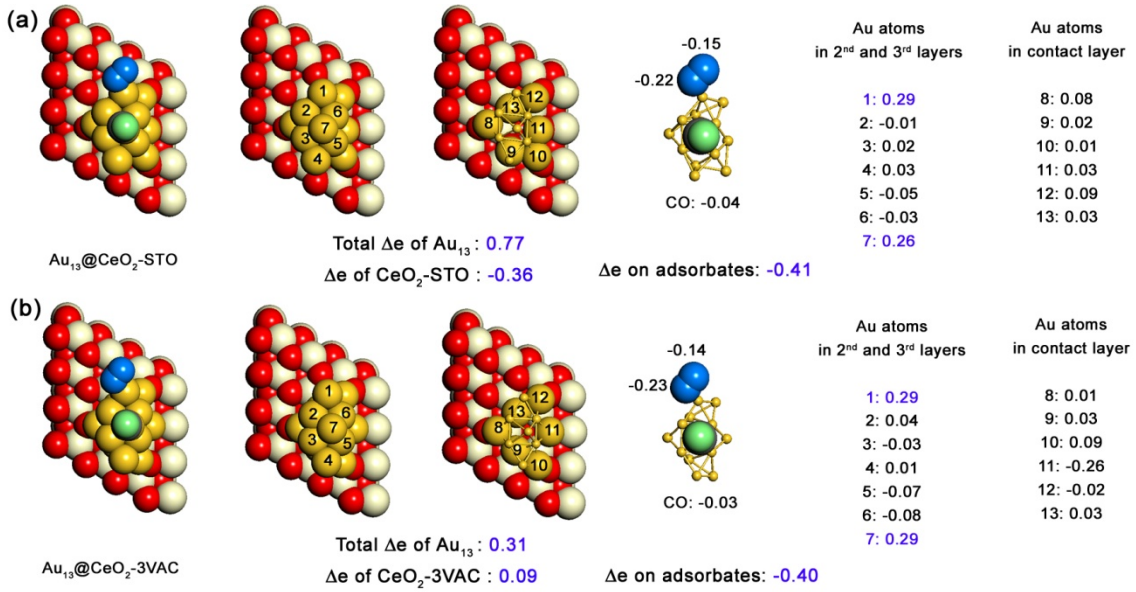

Figure S4. Bader charge analysis on the CO and O_2 adsorption induced charge redistribution in Au_{13}@CeO_2-STO (a) and Au_{13}@CeO_2-STO-3VAC (b). CO and O_2 adsorption leads to electron redistribution over the system. Positive and negative numbers represents the total amount of electron loss and electron accumulation upon CO-O_2 coadsorption, respectively. In both cases, adsorbates draws almost same amount of electrons. Electron rich Au_{13} on CeO_2-3VAC donates 0.31 e to adsorbates and attracts additional 0.09 e from CeO_2-3VAC. It is still highly negatively charged after coadsorption (refer to Bader charge analysis results presented in Figure 6). Au_{13} on CeO_2-STO loses 0.77 e upon adsorption; 0.41 to adsorbates and 0.31 to CeO_2-STO.

XYZ coordinate of selected structures

1) Au_{13}@CeO_2-3VAC, Figure 4e

2) Au_{13}@CeO_2-3VAC, Figure 4h

3) Au_{13}@CeO_2-3VAC with coadsorbed CO-O_2, Stage 1 of Figure 7b

4) Au_{13}@CeO_2-3VAC with CO, Stage1 of Figure 8b

5) Au_{13}@CeO_2-3VAC with coadsorbed CO-O_2, Stage 2 of Figure 10

1) Au_{13}@CeO_2-3VAC, Figure 4e

106

Energy: -28.593021 Ha

Au 8.847086 0.550192 8.847901

Au 7.346923 -1.675426 8.212814

Au 5.888316 3.294870 8.831625

Au 4.407362 1.967952 6.914346

Au 9.670332 -0.882752 6.784854

Au 7.557393 1.927567 10.773582

Au 8.837176 3.313638 8.845514

Au 6.457545 -0.045238 6.056652

Au 10.023122 1.933169 6.618577

Au 5.902610 0.596421 8.771942

Au 7.340021 5.551029 8.238825

Au 9.654708 4.753766 6.791355

Au 6.602706 3.769271 6.106580

Ce 8.853111 7.729618 3.945646

Ce 12.378274 1.923589 3.934585

Ce 5.483043 5.880591 4.009001

Ce 5.411400 1.929603 3.869429

Ce 8.862169 -3.883137 3.943102

Ce 8.851468 -0.066782 3.920154

Ce 2.185391 -0.027418 4.042860

Ce 5.463695 -2.084148 3.938413

Ce 2.228596 7.674020 3.948029

Ce 12.223551 -1.923774 3.953611

Ce 12.186693 -5.764230 3.924140

Ce 2.231447 11.502010 3.957593

Ce 8.882355 3.926492 3.912682

Ce 2.164994 3.889498 3.957489

Ce 5.547030 9.585486 3.947865

Ce 12.229885 5.779450 3.957284

Ce 7.758800 9.599000 0.783800

Ce 11.083900 3.839600 0.783800

Ce 7.758800 1.919800 0.783800

Ce 11.083900 0.000000 0.783800

Ce 1.108400 9.599000 0.783800

Ce 7.758800 5.759400 0.783800

Ce 11.083900 -3.839600 0.783800

Ce 1.108400 13.438600 0.783800

Ce 1.108400 5.759400 0.783800

Ce 4.433600 0.000000 0.783800

Ce 4.433600 11.518800 0.783800

Ce 11.083900 7.679200 0.783800

Ce 1.108400 1.919800 0.783800

Ce 4.433600 7.679200 0.783800

Ce 4.433600 3.839600 0.783800

Ce 7.758800 -1.919800 0.783800

O 10.094003 5.897596 4.955003

O 0.056200 7.694075 4.756371

O 3.152670 5.785640 4.769011

O 10.078078 -2.058289 4.941882

O 3.319308 2.032556 4.985947

O 3.377975 13.266484 4.781849

O 13.274274 -3.790940 4.763331

O 6.637674 11.460803 4.754629

O 13.156928 7.679074 4.780197

O 9.966342 -5.737753 4.739437

O 6.712074 7.851138 4.793427

O 3.309977 9.603399 4.764065

O 0.060231 11.463881 4.784947

O 7.786287 5.788963 3.180273

O 11.110739 3.749574 3.216203

O 11.098265 0.092931 3.222336

O 4.401810 7.738306 3.123117

O 1.122632 9.592866 3.099886

O 7.671068 1.926173 3.279401

O 4.443501 3.794056 3.162547

O 1.070446 5.761701 3.094903

O 7.713986 -1.933953 3.181489

O 4.556676 -0.006096 3.201070

O 11.070450 -3.817608 3.115790

O 7.782788 9.621638 3.092398

O 1.093090 1.977277 3.152520

O 4.436934 11.477730 3.089786

O 1.070602 13.389359 3.139221

O 11.057297 7.668970 3.102574

O 8.867200 7.679200 1.567500

O 2.216800 7.679200 1.567500

O 8.867200 -0.000000 1.567500

O 5.542000 1.919800 1.567500

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O 9.975500 1.919800 0.000000

O 3.325200 5.759400 0.000000

O 6.650400 -0.000000 0.000000

O 3.325200 1.919800 0.000000

O 9.975500 5.759400 0.000000

O 6.650400 7.679200 0.000000

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O 0.000000 3.839600 0.000000

O 9.975500 -1.919800 0.000000

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O 3.325200 -1.919800 0.000000

O 9.975500 9.599000 0.000000

O 3.325200 9.599000 0.000000

O 0.000000 11.518800 0.000000

O 0.000000 0.000000 0.000000

2) Au_{13}@CeO_2-3VAC, Figure 4h

106

Energy: -28.566126 Ha

Au 8.847086 0.550192 8.847901

Au 7.346923 -1.675426 8.212814

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O 6.637674 11.460803 4.754629
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O 8.867200 3.839600 1.567500
O 5.542000 5.759400 1.567500
O 12.192300 1.919800 1.567500
O 2.216800 3.839600 1.567500
O 12.192300 -1.919800 1.567500
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O 2.216800 -0.000000 1.567500
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O 2.216800 11.518800 1.567500
O 12.192300 5.759400 1.567500

O 9.975500 1.919800 0.000000

O 3.325200 5.759400 0.000000

O 6.650400 -0.000000 0.000000

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O 0.000000 3.839600 0.000000

O 9.975500 -1.919800 0.000000

O 6.650400 -3.839600 0.000000

O 3.325200 -1.919800 0.000000

O 9.975500 9.599000 0.000000

O 3.325200 9.599000 0.000000

O 0.000000 11.518800 0.000000

O 0.000000 0.000000 0.000000

3) Au_{13}@CeO_2-STO with coadsorbed CO-O_2, Stage 1 of Figure 7a

113

Energy: -30.337613 Ha

Au 8.450177 0.491319 8.904372

Au 6.590471 -1.507527 9.391242

Au 5.454783 3.584131 9.168418

Au 4.247948 2.358323 6.999421

Au 9.468304 -1.087169 6.919074

Au 7.383834 1.902170 10.960808

Au 8.519007 3.268960 8.823776

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Au 9.654051 1.699407 6.850590

Au 5.480855 0.920872 8.984881

Au 7.306613 5.710943 8.991871

Au 9.205125 5.218313 6.940054

Au 6.671157 4.089452 6.812796

Ce 8.846631 7.708211 3.938407

Ce 12.270171 1.940938 3.922213

Ce 5.508401 5.820224 3.900086

Ce 5.516775 1.905743 3.897387

Ce 8.858190 -3.874081 3.933896

Ce 8.892045 -0.029889 3.911170

Ce 2.196814 -0.025960 4.036082

Ce 5.500417 -1.986300 3.932355

Ce 2.220170 7.692181 3.930173

Ce 12.226295 -1.928388 3.936144

Ce 12.188161 -5.770491 3.929749

Ce 2.226283 11.511143 3.942882

Ce 8.890315 3.849882 3.970402

Ce 2.191377 3.880128 3.931413

Ce 5.532925 9.596345 3.931994

Ce 12.227085 5.769097 3.947286

Ce 7.758800 9.599000 0.783800

Ce 11.083900 3.839600 0.783800

Ce 7.758800 1.919800 0.783800

Ce 11.083900 0.000000 0.783800

Ce 1.108400 9.599000 0.783800

Ce 7.758800 5.759400 0.783800

Ce 11.083900 -3.839600 0.783800

Ce 1.108400 13.438600 0.783800

Ce 1.108400 5.759400 0.783800

Ce 4.433600 0.000000 0.783800

Ce 4.433600 11.518800 0.783800

Ce 11.083900 7.679200 0.783800

Ce 1.108400 1.919800 0.783800

Ce 4.433600 7.679200 0.783800

Ce 4.433600 3.839600 0.783800

Ce 7.758800 -1.919800 0.783800

O 10.034532 5.885212 5.031457

O 10.117483 1.865285 4.789250

O 6.504905 3.848681 4.735837
O 0.027353 7.680804 4.719520
O 3.321293 5.790022 4.715376
O 10.006365 -1.979179 4.889423
O 6.604003 -0.050790 4.853588
O 3.401787 2.067066 5.038403
O 3.407552 13.293622 4.775641
O 13.290071 -3.795458 4.753448
O 6.650643 11.493784 4.718182
O 13.154137 7.699649 4.770774
O 9.955889 -5.745673 4.729591
O 6.610248 7.713427 4.741147
O 3.330292 9.577123 4.736355
O 0.037656 11.476922 4.778888
O 7.748602 5.824556 3.144073
O 11.148918 3.873245 3.137545
O 11.061309 -0.038649 3.126884
O 4.426752 7.688739 3.097768
O 1.127275 9.596611 3.103816
O 7.731650 1.823333 3.170584
O 4.399596 3.816235 3.102639
O 1.107413 5.761203 3.112329
O 7.791955 -1.903658 3.145204
O 4.483424 0.027572 3.149736
O 11.070873 -3.819138 3.124729
O 7.760377 9.596563 3.113785
O 1.118880 1.984877 3.159022
O 4.440425 11.487687 3.092129
O 1.081756 13.393189 3.145348
O 11.038570 7.651734 3.113437
O 8.867200 7.679200 1.567500
O 2.216800 7.679200 1.567500
O 8.867200 -0.000000 1.567500
O 5.542000 1.919800 1.567500
O 8.867200 3.839600 1.567500
O 5.542000 5.759400 1.567500
O 12.192300 1.919800 1.567500
O 2.216800 3.839600 1.567500
O 12.192300 -1.919800 1.567500
O 5.542000 -1.919800 1.567500
O 2.216800 -0.000000 1.567500
O 12.192300 -5.759400 1.567500
O 8.867200 -3.839600 1.567500
O 5.542000 9.599000 1.567500
O 2.216800 11.518800 1.567500
O 12.192300 5.759400 1.567500
O 9.975500 1.919800 0.000000
O 3.325200 5.759400 0.000000
O 6.650400 -0.000000 0.000000
O 3.325200 1.919800 0.000000
O 9.975500 5.759400 0.000000
O 6.650400 7.679200 0.000000
O 6.650400 3.839600 0.000000
O 0.000000 7.679200 0.000000
O 0.000000 3.839600 0.000000
O 9.975500 -1.919800 0.000000
O 6.650400 -3.839600 0.000000
O 3.325200 -1.919800 0.000000
O 9.975500 9.599000 0.000000
O 3.325200 9.599000 0.000000
O 0.000000 11.518800 0.000000
O 0.000000 0.000000 0.000000
O 6.467087 7.272113 10.207655
O 7.377399 8.186403 10.335931
O 7.410885 2.091311 14.044213
C 7.174409 2.121437 12.915096

4) Au_{13}@CeO_2-3VAC with CO, Stage1 of Figure 8b

111

Energy: -29.963359 Ha

Au 8.547435 0.483510 8.896756

Au 6.762057 -1.586663 9.349606

Au 5.552314 3.390996 9.153130

Au 4.238862 2.223070 7.007390

Au 9.539366 -0.934836 6.846067

Au 7.252976 1.862796 10.867601

Au 8.466239 3.334845 8.885246

Au 6.658800 -0.570424 6.884275

Au 9.684801 1.888562 6.896657

Au 5.367930 0.718354 8.997816

Au 7.148195 5.762772 8.984613

Au 9.357578 4.943018 6.902492

Au 6.583036 4.223832 6.828959

Ce 8.847060 7.702268 3.938136

Ce 12.263491 1.941067 3.922698

Ce 5.508659 5.816535 3.903196

Ce 5.512520 1.913044 3.904596

Ce 8.852290 -3.876978 3.937055

Ce 8.888001 -0.013343 3.898265

Ce 2.198323 -0.022354 4.033580

Ce 5.502603 -1.983528 3.935484

Ce 2.221471 7.691914 3.928784

Ce 12.232859 -1.922685 3.940761

Ce 12.188024 -5.769523 3.930823

Ce 2.224898 11.512001 3.941649

Ce 8.885070 3.848185 3.955510

Ce 2.194533 3.875464 3.931870

Ce 5.532260 9.594512 3.929258

Ce 12.224414 5.767529 3.946176

Ce 7.758800 9.599000 0.783800

Ce 11.083900 3.839600 0.783800

Ce 7.758800 1.919800 0.783800

Ce 11.083900 0.000000 0.783800

Ce 1.108400 9.599000 0.783800

Ce 7.758800 5.759400 0.783800

Ce 11.083900 -3.839600 0.783800

Ce 1.108400 13.438600 0.783800

Ce 1.108400 5.759400 0.783800

Ce 4.433600 0.000000 0.783800

Ce 4.433600 11.518800 0.783800

Ce 11.083900 7.679200 0.783800

Ce 1.108400 1.919800 0.783800

Ce 4.433600 7.679200 0.783800

Ce 4.433600 3.839600 0.783800

Ce 7.758800 -1.919800 0.783800

O 10.025039 5.872215 5.008426

O 10.107328 1.852861 4.775971

O 6.517384 3.853012 4.750940

O 0.024896 7.679056 4.721980

O 3.319410 5.792164 4.712783

O 10.005266 -1.951801 4.946220

O 6.627433 -0.048734 4.849766

O 3.394449 2.065025 4.997913

O 3.407855 13.294711 4.771795

O 13.287934 -3.795235 4.755355

O 6.655833 11.492804 4.722185

O 13.151329 7.701561 4.768215

O 9.952440 -5.744083 4.736699

O 6.613481 7.716219 4.745400

O 3.331252 9.577409 4.737271

O 0.034679 11.477357 4.778711

O 7.742016 5.823613 3.139467

O 11.149100 3.870825 3.132572

O 11.062788 -0.044001 3.122028

O 4.428655 7.688820 3.098607

O 1.125681 9.595471 3.104707

O 7.725040 1.832521 3.158727
O 4.406245 3.821839 3.103253
O 1.106301 5.762351 3.112495
O 7.800558 -1.908084 3.143233
O 4.490759 0.026494 3.152358
O 11.059652 -3.804481 3.135644
O 7.761328 9.597335 3.114039
O 1.111215 1.984834 3.156018
O 4.444188 11.488213 3.093463
O 1.080358 13.392997 3.144834
O 11.036804 7.655953 3.114205
O 8.867200 7.679200 1.567500
O 2.216800 7.679200 1.567500
O 8.867200 -0.000000 1.567500
O 5.542000 1.919800 1.567500
O 8.867200 3.839600 1.567500
O 5.542000 5.759400 1.567500
O 12.192300 1.919800 1.567500
O 2.216800 3.839600 1.567500
O 12.192300 -1.919800 1.567500
O 5.542000 -1.919800 1.567500
O 2.216800 -0.000000 1.567500
O 12.192300 -5.759400 1.567500
O 8.867200 -3.839600 1.567500
O 5.542000 9.599000 1.567500
O 2.216800 11.518800 1.567500
O 12.192300 5.759400 1.567500
O 9.975500 1.919800 0.000000
O 3.325200 5.759400 0.000000
O 6.650400 -0.000000 0.000000
O 3.325200 1.919800 0.000000
O 9.975500 5.759400 0.000000
O 6.650400 7.679200 0.000000
O 6.650400 3.839600 0.000000
O 0.000000 7.679200 0.000000
O 0.000000 3.839600 0.000000
O 9.975500 -1.919800 0.000000
O 6.650400 -3.839600 0.000000
O 3.325200 -1.919800 0.000000
O 9.975500 9.599000 0.000000
O 3.325200 9.599000 0.000000
O 0.000000 11.518800 0.000000
O 0.000000 0.000000 0.000000
O 6.890388 8.592468 10.219115
C 7.063666 7.528587 9.807607

5) Au_{13}@CeO_2-3VAC with coadsorbed CO-O_2, Stage 2 of Figure 10

110

Energy: -29.527637 Ha

Au 8.876803 0.683994 8.834958
Au 7.471764 -1.622317 8.147891
Au 5.029123 3.054010 9.303880
Au 4.310049 1.793576 6.932971
Au 9.748005 -0.759050 6.769466
Au 7.507563 2.136612 10.702730
Au 8.728647 3.457041 8.723149
Au 6.498956 -0.022102 5.991017
Au 10.054661 2.032834 6.555330
Au 6.068755 0.719751 8.659811
Au 7.253835 5.574468 7.958041
Au 9.643455 4.901648 6.764714
Au 6.675714 3.431488 6.175486
Ce 8.860337 7.737776 3.934882
Ce 12.381740 1.922864 3.933937
Ce 5.479295 5.891313 4.159533
Ce 5.406811 1.922846 3.849026
Ce 8.864902 -3.878365 3.945523

Ce 8.865030 -0.060856 3.908320
Ce 2.188645 -0.033609 4.046549
Ce 5.467165 -2.086630 3.933804
Ce 2.234093 7.672361 3.949838
Ce 12.228389 -1.918093 3.954252
Ce 12.190277 -5.763422 3.924507
Ce 2.237172 11.498806 3.955721
Ce 8.880813 3.915065 3.909598
Ce 2.159129 3.885295 3.949682
Ce 5.552353 9.584054 3.950498
Ce 12.244151 5.778408 3.949084
Ce 7.758800 9.599000 0.783800
Ce 11.083900 3.839600 0.783800
Ce 7.758800 1.919800 0.783800
Ce 11.083900 0.000000 0.783800
Ce 1.108400 9.599000 0.783800
Ce 7.758800 5.759400 0.783800
Ce 11.083900 -3.839600 0.783800
Ce 1.108400 13.438600 0.783800
Ce 1.108400 5.759400 0.783800
Ce 4.433600 0.000000 0.783800
Ce 4.433600 11.518800 0.783800
Ce 11.083900 7.679200 0.783800
Ce 1.108400 1.919800 0.783800
Ce 4.433600 7.679200 0.783800
Ce 4.433600 3.839600 0.783800
Ce 7.758800 -1.919800 0.783800
O 10.137557 5.906531 4.932877
O 0.063460 7.697086 4.758401
O 3.114386 5.751913 4.744709
O 10.090876 -2.020125 4.972576
O 3.322748 2.009981 5.010031
O 3.385462 13.265437 4.783385
O 13.272079 -3.798276 4.759570
O 6.641845 11.463746 4.755352
O 13.164137 7.680827 4.778785
O 9.973866 -5.727429 4.737273
O 6.769389 7.875737 4.776061
O 3.308330 9.614974 4.743815
O 0.065172 11.464559 4.781918
O 7.772806 5.772057 3.220140
O 11.107211 3.743043 3.216339
O 11.105564 0.088159 3.212693
O 4.419783 7.717251 3.157347
O 1.123906 9.591174 3.097029
O 7.672376 1.925491 3.245794
O 4.458500 3.796488 3.189237
O 1.059876 5.764401 3.087607
O 7.721905 -1.934521 3.182535
O 4.552031 -0.013579 3.193647
O 11.063862 -3.804653 3.121329
O 7.790105 9.638546 3.084643
O 1.098908 1.973379 3.149739
O 4.443386 11.477592 3.086688
O 1.079218 13.388054 3.134960
O 11.065401 7.677188 3.095242
O 8.867200 7.679200 1.567500
O 2.216800 7.679200 1.567500
O 8.867200 -0.000000 1.567500
O 5.542000 1.919800 1.567500
O 8.867200 3.839600 1.567500
O 5.542000 5.759400 1.567500
O 12.192300 1.919800 1.567500
O 2.216800 3.839600 1.567500
O 12.192300 -1.919800 1.567500
O 5.542000 -1.919800 1.567500
O 2.216800 -0.000000 1.567500
O 12.192300 -5.759400 1.567500

O 8.867200 -3.839600 1.567500

O 5.542000 9.599000 1.567500

O 2.216800 11.518800 1.567500

O 12.192300 5.759400 1.567500

O 9.975500 1.919800 0.000000

O 3.325200 5.759400 0.000000

O 6.650400 -0.000000 0.000000

O 3.325200 1.919800 0.000000

O 9.975500 5.759400 0.000000

O 6.650400 7.679200 0.000000

O 6.650400 3.839600 0.000000

O 0.000000 7.679200 0.000000

O 0.000000 3.839600 0.000000

O 9.975500 -1.919800 0.000000

O 6.650400 -3.839600 0.000000

O 3.325200 -1.919800 0.000000

O 9.975500 9.599000 0.000000

O 3.325200 9.599000 0.000000

O 0.000000 11.518800 0.000000

O 0.000000 0.000000 0.000000

O 5.556700 6.853654 7.809588

O 4.880909 6.766053 6.680995

O 3.876979 5.423913 10.922458

C 4.349779 4.587370 10.290511