Supplementary information:

Band Gap Modulation of $SrTiO_3$ upon CO_2 Adsorption

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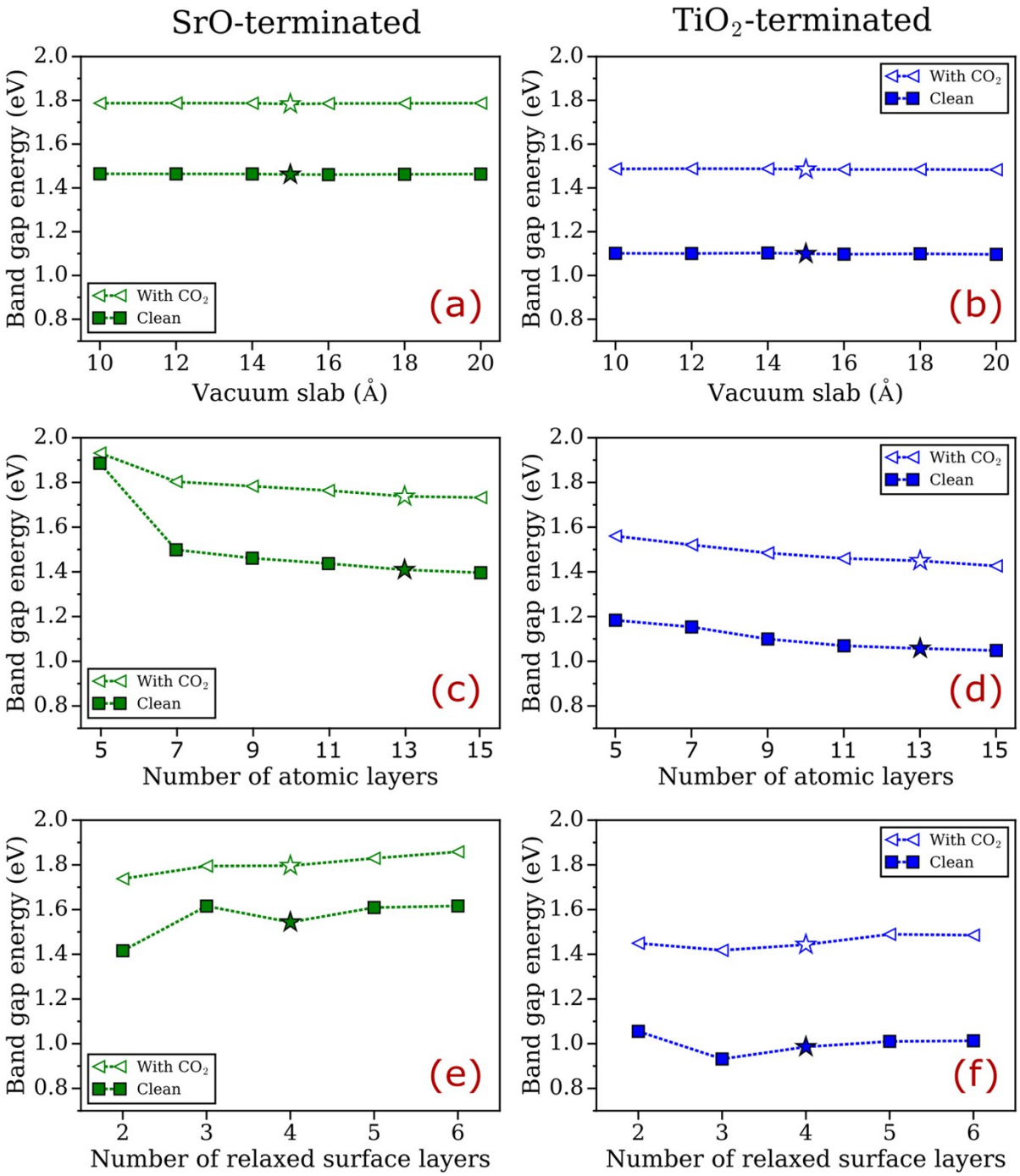


Figure S1. Convergence of the computed band gap energy with (a,b) thickness of vacuum slab, (c,d) number of atomic layers, and (e,f) number of relaxed surface layers for modeled (a,c,e) SrO-terminated and (b,d,f) TiO_2-terminated $SrTiO_3$(001) slabs. Star markers represent default values of X used in all other calculations. (a-d) are computed for $SrTiO_3$(001) slabs with two relaxed surface layers. Other model parameters are described in the methods.

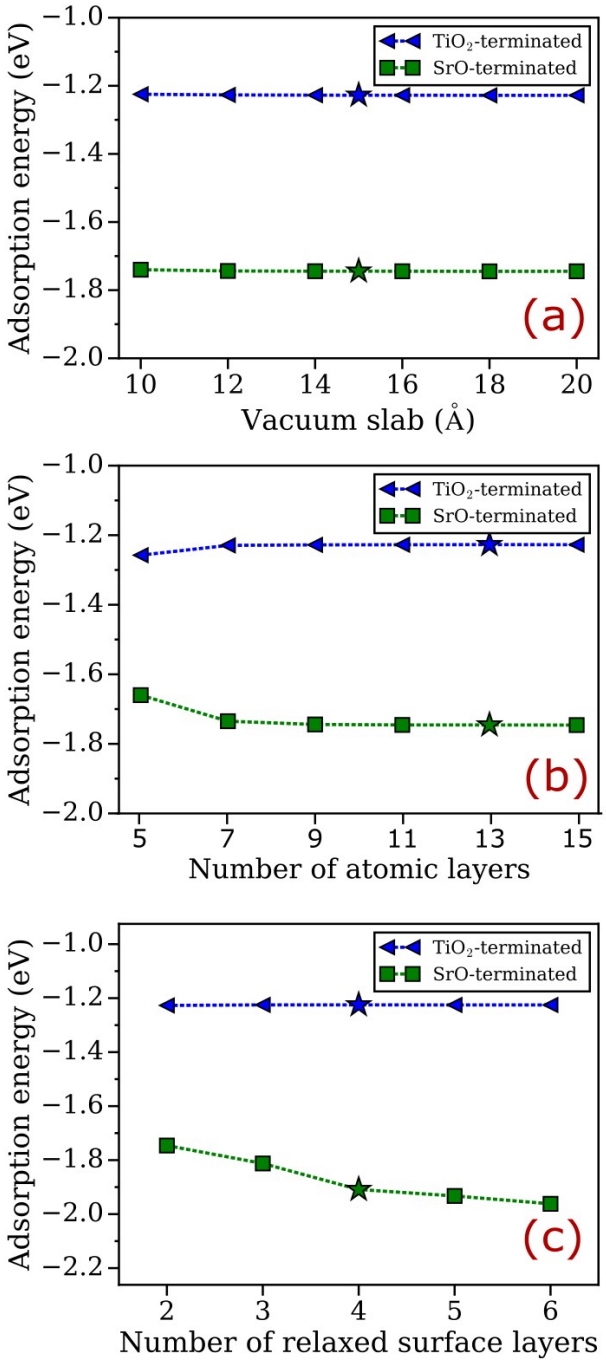


Figure S2. Convergence of the computed CO_2 adsorption energy with (a) thickness of vacuum slab, (b) number of atomic layers, and (c) number of relaxed surface layers for modeled $SrTiO_3$(001) slab. Star markers represent default values of X used in all other calculations. (a,b) are computed for $SrTiO_3$(001) slabs with two relaxed surface layers. Other model parameters are described in the methods.

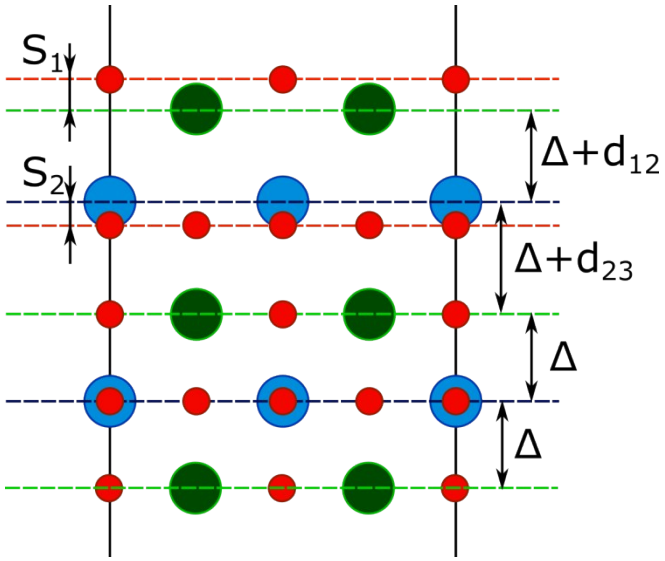


Figure S3. Illustration of the structure relaxation parameters used in this work. Δ represents the interplanar distance in bulk $SrTiO_3$ ($2\Delta = 3.94$ Å). Green, blue, and red circles represent Sr, Ti, and O ions, respectively.

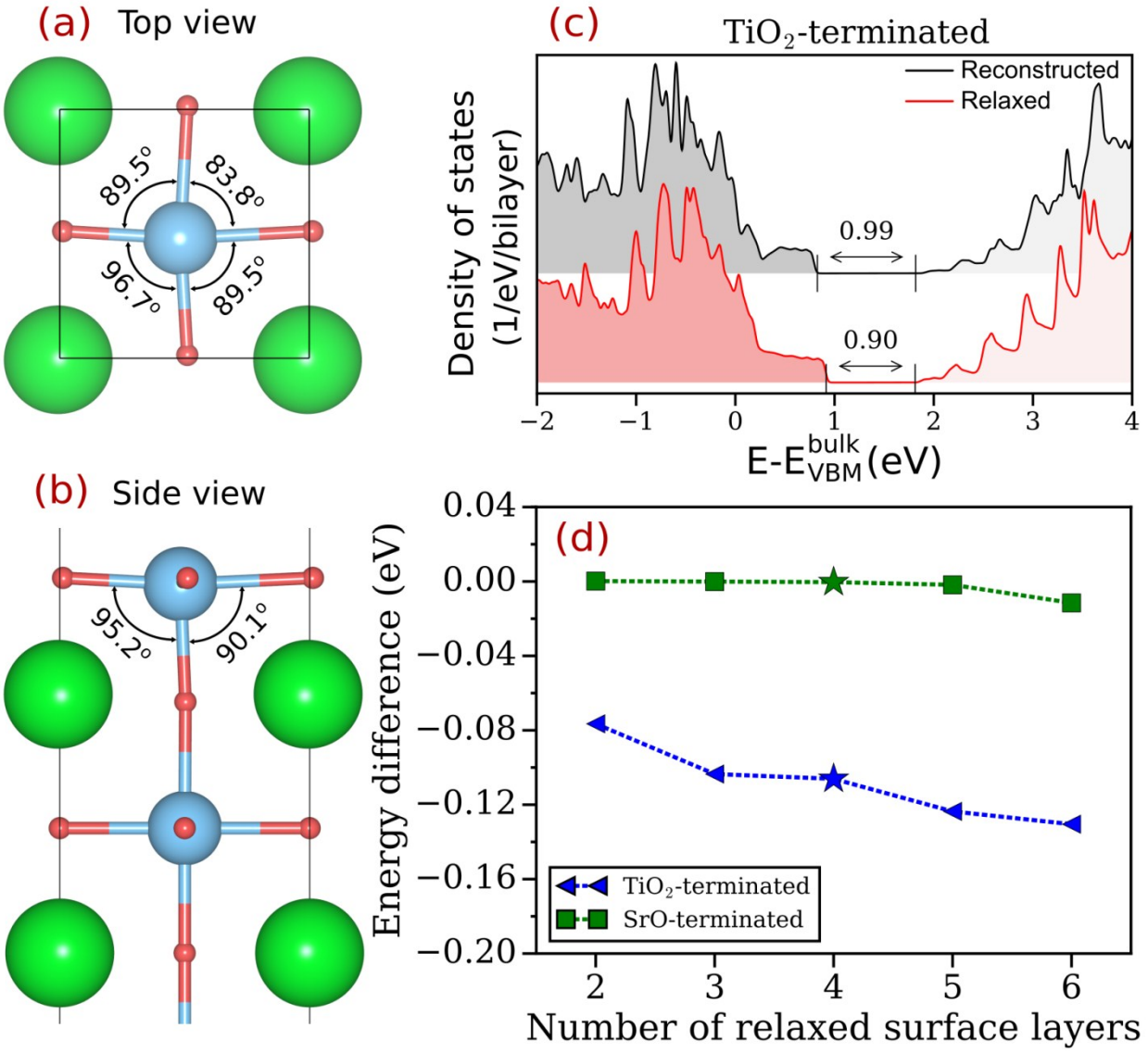


Figure S4. Illustration of the surface reconstruction on TiO_2-terminated $SrTiO_3$(001) surface. (a) top view and (b) side view of the reconstructed surface. (c) Comparison of electronic structures of relaxed (not reconstructed) and reconstructed surfaces. (d) Energy difference per 2×2 surface supercell between relaxed (not reconstructed) and reconstructed $SrTiO_3$(001) surface vs. number of relaxed surface layers. Star markers represent default values of X used in all other calculations.

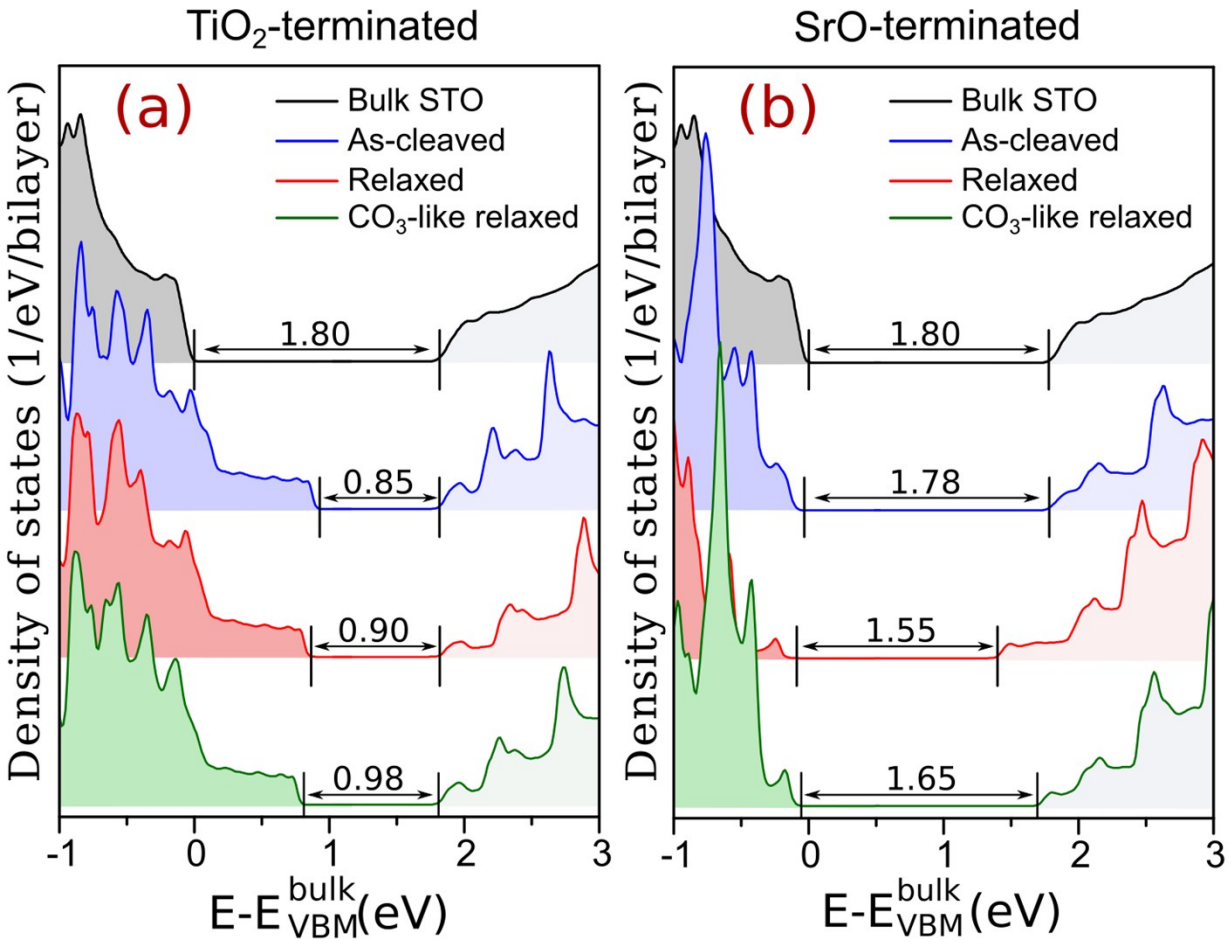


Figure S5. Formation and evolution of the surface states at (a) TiO_2-terminated and (b) SrO-terminated $SrTiO_3$(001). Black, red, blue, and green curves represent densities of states for bulk $SrTiO_3$, as-cleaved, relaxed (not reconstructed), and "CO_3-like relaxed" surfaces, respectively. Structure parameters of "CO_3-like relaxed" surface are identical to those of the $SrTiO_3$(001) containing one adsorbed CO_2 molecule per 2×2 surface supercell (see Table S3). Strokes and numbers represent valence band maximum (VBM), conduction band minimum (CBM), and band gap energies of $SrTiO_3$(001) slabs.

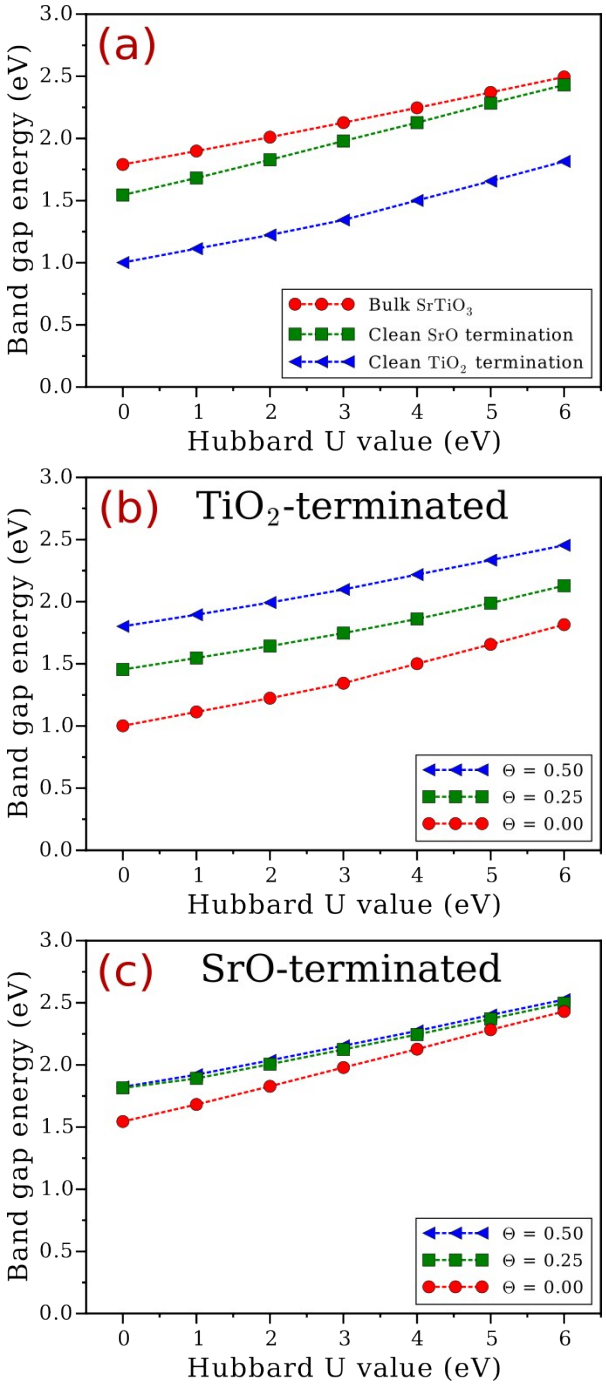
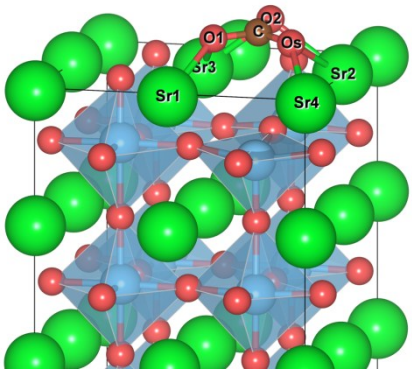


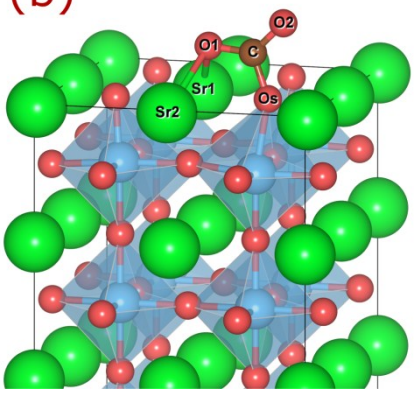
Figure S6. (a) Band gap energies of bulk $SrTiO_3$ and clean TiO_2- and SrO-terminated $SrTiO_3$(001) surfaces as functions of Hubbard U value. Band gap energies of (b) TiO_2- and (c) SrO-terminated $SrTiO_3$(001) surfaces as functions of Hubbard U value for slab systems containing zero (Θ = 0.00), one (Θ = 0.25), and two (Θ = 0. 50) adsorbed CO_2 molecules per 2×2 surface supercell. Here, cutoff energy of 400 eV for plane wave basis sets was used for all DFT+U calculations.

(a)



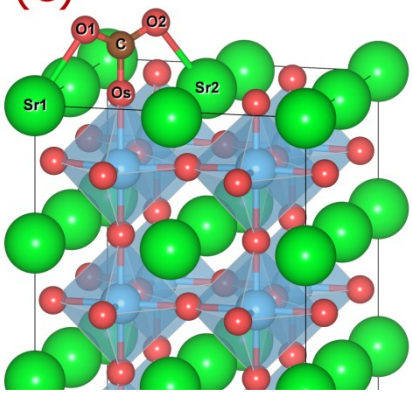
C-O1, C-O2, C-O_S	1.30 Å
O1-Sr1, O_S-Sr4	2.44 Å
O1-Sr3, O_S-Sr2	2.65 Å
O2-Sr3, O2-Sr2	2.56 Å
∠(O1-C-O2)	122°
∠(O1-C-O2), ∠(O2-C-O_S)	119°

(b)

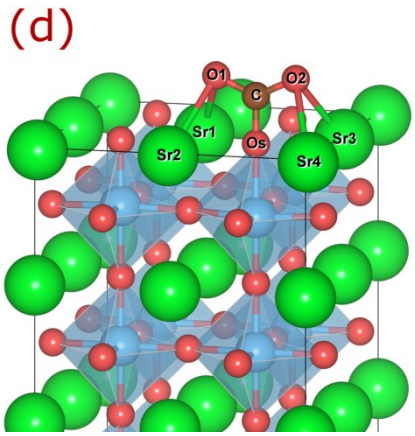


C-O1	1.30 Å
C-O2	1.25 Å
C-O_S	1.38 Å
O1-Sr1, O1-Sr2	2.63 Å
∠(O1-C-O2)	129°
∠(O1-C-O_S)	115°
∠(O2-C-O_S)	117°

(c)



C-O1, C-O2	1.27 Å
C-O_S	1.39 Å
O1-Sr1, O2-Sr2	2.60 Å
∠(O1-C-O2)	129°
∠(O1-C-O_S), ∠(O2-C-O_S)	115°



C-O1, C-O2	1.27 Å
C-O_S	1.37 Å
O1-Sr1, O1-Sr2, O2-Sr3, O2-Sr4	2.91 Å
∠(O1-C-O2)	130°
∠(O1-C-O_S), ∠(O2-C-O_S)	115°

Figure S7. Metastable CO_2 adsorption configurations on SrO-terminated $SrTiO_3$(001) surface. The computed adsorption energies for (a), (b), (c), and (d) are 0.06, 0.47, 0.49, and 0.54 eV higher as compared to the most stable adsorption configuration presented in Fig. 2a.

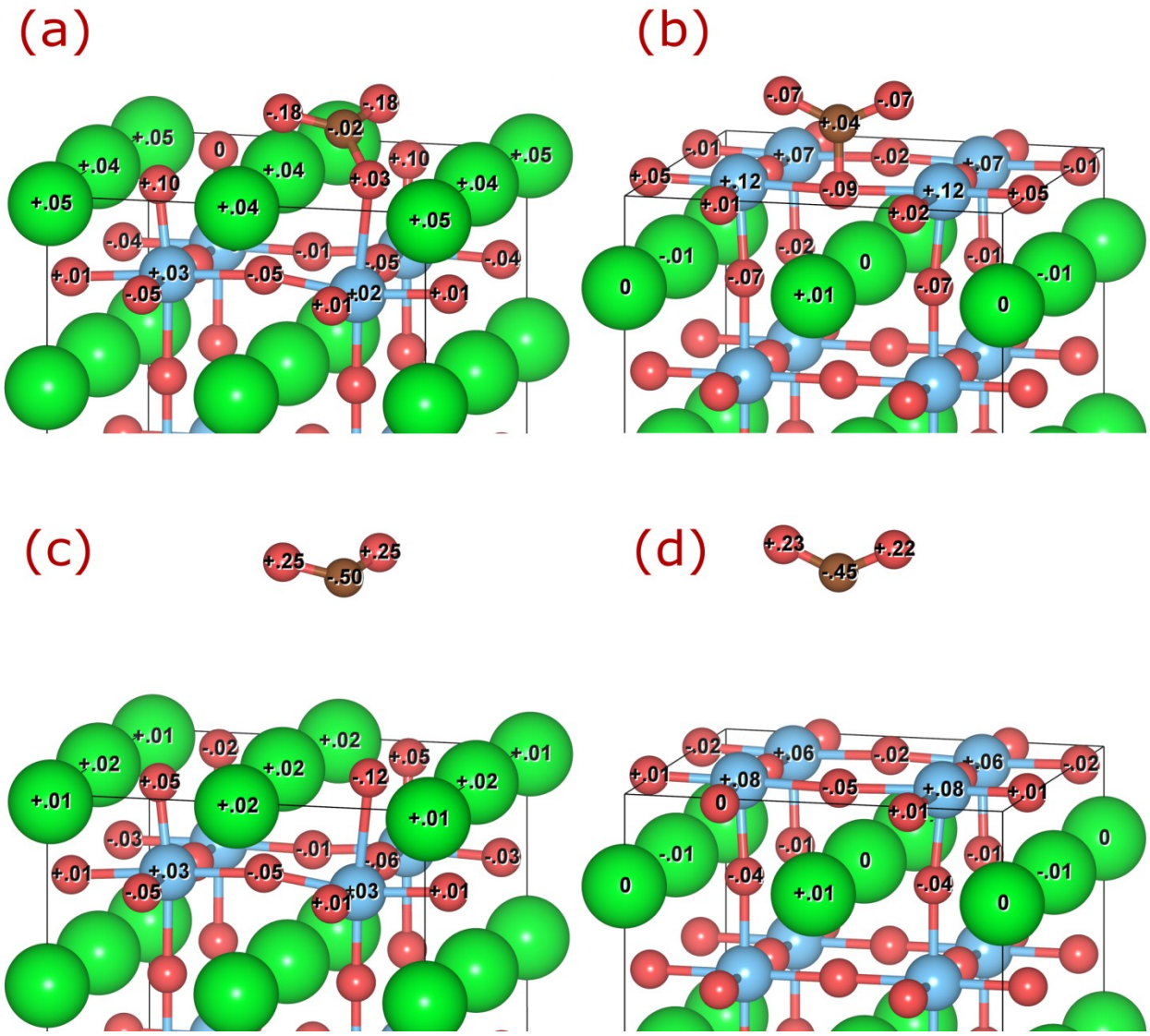


Figure S8. Bader charge transfers imposed by CO_2 adsorption on (a) SrO-terminated and (b) TiO_2-terminated $SrTiO_3$(001) surfaces. Bader charge redistribution within the separated as-deformed CO_2 molecules and (c) SrO-terminated as well as (d) TiO_2-terminated $SrTiO_3$(001) surfaces with respect to the free CO_2 molecule and clean $SrTiO_3$(001) slabs. The Bader charge transfers of as-deformed CO_2 molecules and $SrTiO_3$(001) slabs are computed separately.

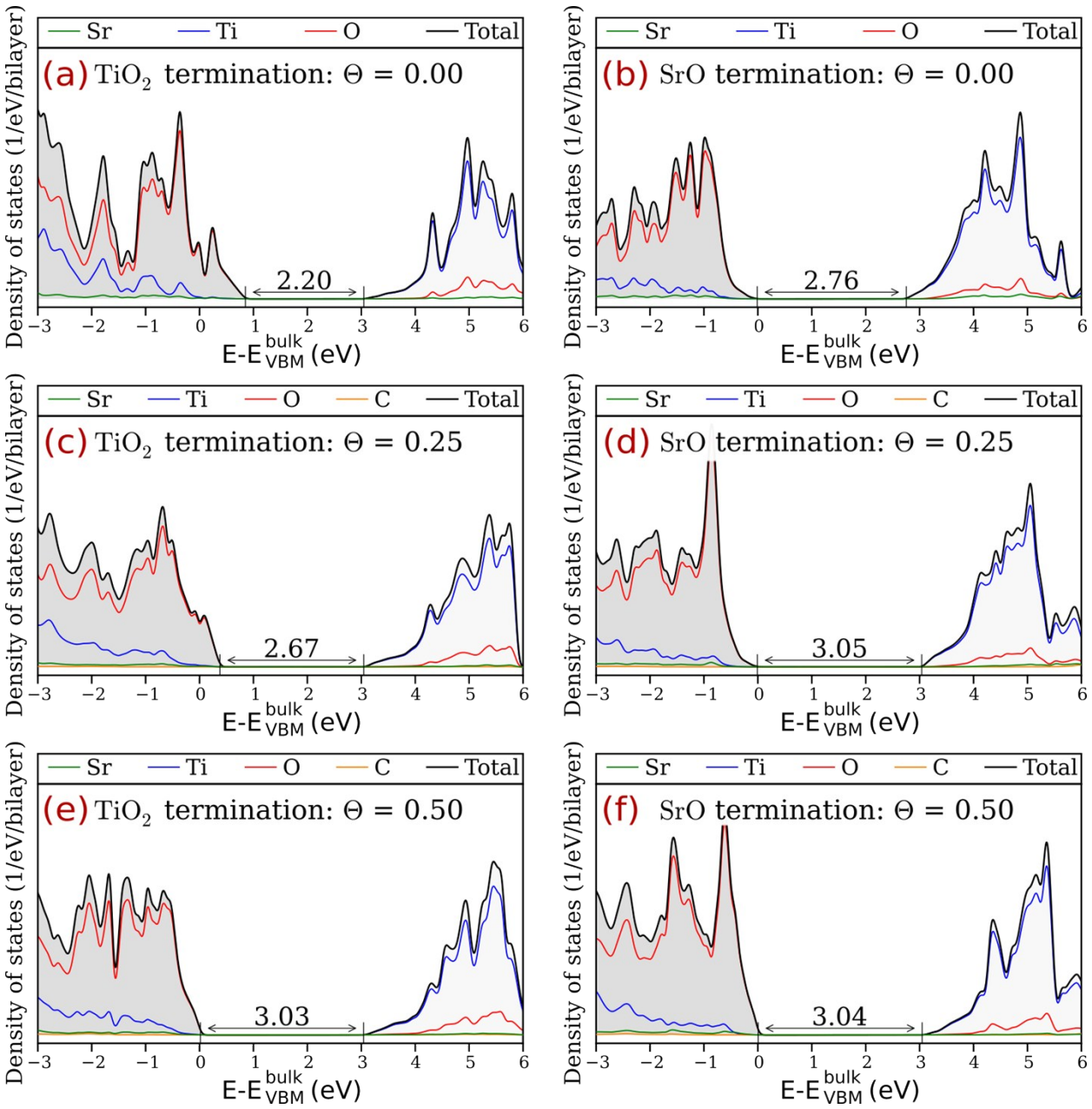


Figure S9. Projected densities of states computed using hybrid HSE functional for two top layers of (a,c,e) TiO_2-terminated and (b,d,f) SrO-terminated $SrTiO_3$(001) slabs containing (a,b) zero (Θ=0.00), (c,d) one (Θ=0.25), and (e,f) two (Θ=0.50) adsorbed CO_2 molecules per 2×2 surface supercell. For all calculations, we employ 2×2×1 Monkhorst Pack grid and cutoff energy of 400 eV for plane wave basis sets with $3d^24s^2$ electrons of Ti treated explicitly. The calculations are carried out on the optimized geometries obtained from the PBE relaxations.

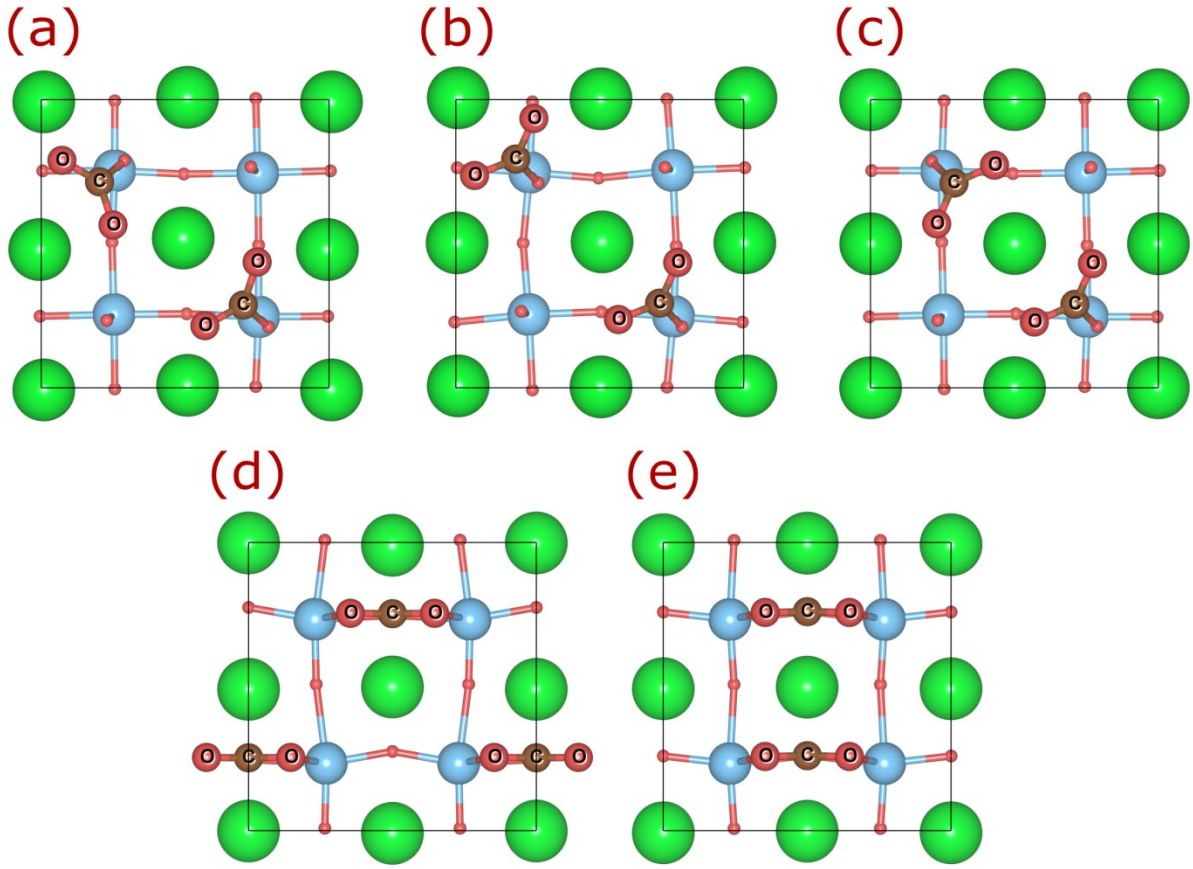


Figure S10. Different CO_2 coverage modes corresponding to $\Theta = 0.5$ on (a-c) SrO-terminated and (d,e) TiO_2-terminated $SrTiO_3$(001). (a) and (d) are the most stable modes. The computed adsorption energies for (b), (c), and (e) modes are 0.07, 0.14, and 0.03 eV/molecule higher as compared to the most stable configuration.

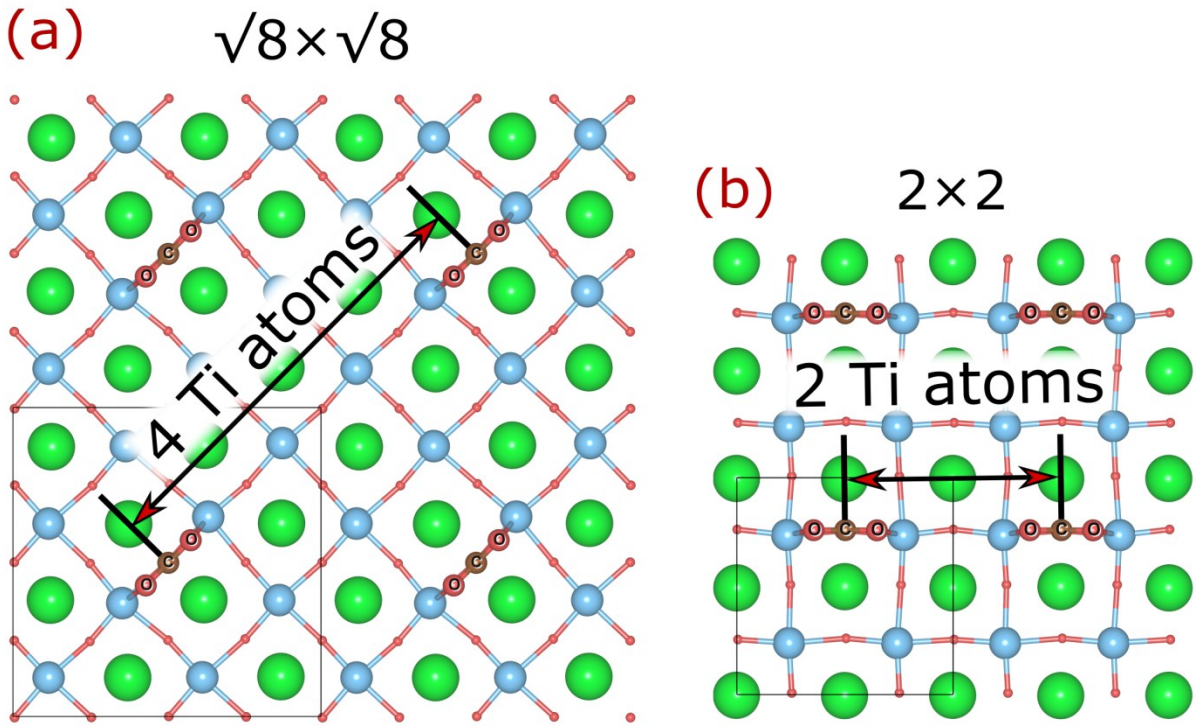


Figure S11. Illustration of "supercell size along O1-O2" term used in this manuscript. O1-O2 refers to a vector connecting O atoms of the adsorbed CO_2 molecule. (a) and (b) illustrate the supercell size along O1-O2 for √8×√8 and 2×2 supercells, respectively.

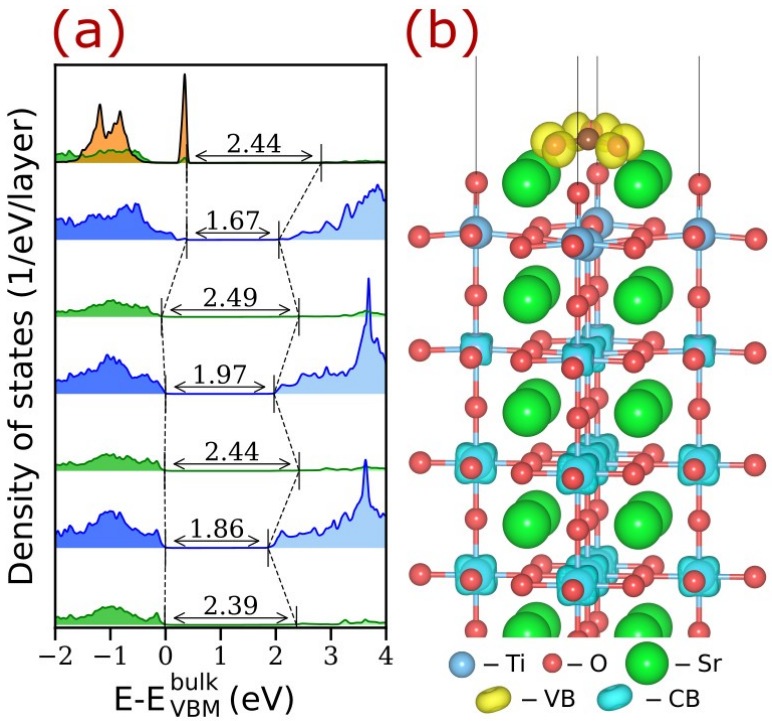


Figure S12. Computed electronic structures of CO_3-like complex adsorbed on the surface oxygen vacancy in $\sqrt{2}\times\sqrt{2}$ SrO-terminated $SrTiO_3(001)$ system. (a) Layer-resolved density of states (LDOS). Orange, green, and blue curves represent population densities for the adsorbed CO_3-like complex, SrO, and TiO_2 layers, respectively. Numbers illustrate effective band gap energies of each atomic layer computed from LDOS neglecting the population densities below 0.1 1/eV/layer. (b) Partial charge density distribution at VB (yellow) and CB (blue) of the $SrTiO_3$ slabs. The computed CO_2 adsorption energy for this system is 0.31 eV/molecule higher as compared to the most stable configuration with the same coverage ($\Theta = 0.5$).

Table S1. Sizes of supercells, Γ-centered Monkhorst-Pack grids used in the calculations, corresponding CO_2 coverages, and supercell sizes along O1-O2 atoms of the CO_2 molecule adsorbed on TiO_2-terminated $SrTiO_3$(001) surface; see Fig. S11 for more details. The systems are labeled by their lateral dimensions in units of lattice constant. "2×2/2" refers to the systems containing two CO_2 molecules per 2×2 surface supercell (see Fig. S10).

Supercell size	Monkhorst-Pack grid	CO_2 coverage	Supercell size along O1-O2
√2×√2	7×7×1	0.5	–
1×2	5×10×1	0.5	2
1×3	3×10×1	0.333	3
1×4	2×10×1	0.25	4
1×5	1×10×1	0.2	5
2×2/2	5×5×1	0.5	2
2×2	5×5×1	0.25	2
2×3	3×5×1	0.167	3
2×4	2×5×1	0.125	4
√8×√8	3×3×1	0.125	4
3×3	3×3×1	0.111	3

Table S2. Structure parameters for the clean $SrTiO_3$(001) surfaces. The values are given in percent of the lattice constant.

	SrO-terminated $SrTiO_3$(001)	TiO_2-terminated $SrTiO_3$(001)
S_1, %	5.63	2.45
S_2, %	-1.13	-3.35
d_{12}, %	-6.87	-6.23
d_{23}, %	3.11	4.16

Table S3. Structure parameters for the $SrTiO_3(001)$ surfaces containing one adsorbed CO_2 molecule per 2×2 surface supercell. The values are given in percent of the lattice constant.

	CO_2 on SrO-terminated $SrTiO_3(001)$	CO_2 on TiO_2-terminated $SrTiO_3(001)$
S_1, %	4.33	0.47
S_2, %	-0.01	-1.59
d_{12}, %	-2.89	-3.39
d_{23}, %	2.01	2.05

Table S4. Summary of the computational results. The stability (last column) indicates whether the system has the lowest CO_2 adsorption energy for a given CO_2 coverage.

Surface	Coverage	System	Figure		Adsorption energy (eV)	Band gap (eV)	C-Os bond length (Å)	C-O1 (C-O2) bond lengths (Å)	∠(O1-C-O2) (°)	Stable Yes/No
SrO-terminated $SrTiO_3$(001)	0.5	√2×√2	2a	-	-1.39	1.82	1.36	1.27	123.9	No
			S7a		-1.15	1.43	1.30	1.30 (1.29)	119.3	No
		2×2/2	2a	S10a	-1.46	1.84	1.36	1.27	124.3	Yes
				S10b	-1.39	1.84	1.36	1.27	124.0	No
				S10c	-1.32	1.79	1.36	1.28	124.1	No
	0.25	2×2	2a	-	-1.94	1.82	1.33	1.29	122.2	Yes
			S7a		-1.88	1.83	1.30	1.30	119.0	No
			S7b		-1.47	1.75	1.38	1.30 (1.25)	128.8	No
			S7c		-1.45	1.72	1.39	1.27	129.3	No
			S7d		-1.40	1.72	1.37	1.27	130.4	No
	0.167	2×3	S7a		-2.10	1.81	1.30	1.30	119.0	Yes
		3×2			-2.09	1.82	1.30	1.30	119.0	No
	0.125	√8×√8			-2.25	1.74	1.30	1.30	119.0	Yes
	0.111	3×3			-2.28	1.74	1.30	1.30	119.0	Yes
	0	2×2	1f		-	1.55	-	-	-	-
TiO_2-terminated $SrTiO_3$(001)	0.5	1×2	2b	-	-1.16	1.80	1.37	1.27	131.4	No
		2×2/2		S10d	-1.19	1.85	1.37	1.27	130.8	Yes
				S10e	-1.16	1.80	1.37	1.27	131.4	No
	0.333	1×3		-	-1.42	1.61	1.36	1.27	130.0	Yes
	0.25	1×4			-1.52	1.37	1.36	1.27	129.6	Yes
		2×2			-1.24	1.50	1.37	1.27	130.8	No
	0.2	1×5			-1.56	1.24	1.35	1.27	129.4	Yes
	0.167	2×3			-1.47	1.32	1.35	1.27	129.5	Yes
	0.125	2×4			-1.55	1.19	1.35	1.27	129.2	No
		√8×√8			-1.57	1.19	1.35	1.27	129.1	Yes
	0.111	3×3			-1.49	1.22	1.35	1.27	129.5	Yes
	0	2×2	1b		-	0.99	-	-	-	-

Most stable CO_2 adsorption configuration on TiO_2-terminated $SrTiO_3$(001) surface, as illustrated in Fig. 2b.

```
_chemical_name_common                  'Sr24 Ti28 C2 O84 '
_cell_length_a                         7.88820
_cell_length_b                         7.88820
_cell_length_c                         38.64670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
 Sr  0.996244    0.996000    0.049046
 Sr  0.997719    0.487818    0.050107
 Sr  0.496407    0.994011    0.048686
 Sr  0.496961    0.494732    0.048335
 Sr  0.000000    0.000000    0.357185
 Sr  0.000000    0.500000    0.357185
 Sr  0.500000    0.000000    0.357185
 Sr  0.500000    0.500000    0.357185
 Sr  0.497341    0.499463    0.459599
 Sr  0.497436    0.993864    0.459526
 Sr  0.997303    0.499078    0.459529
 Sr  0.997158    0.994234    0.459571
 Sr  0.496961    0.494732    0.563983
 Sr  0.496407    0.994011    0.563632
 Sr  0.997719    0.487818    0.562210
 Sr  0.996244    0.996000    0.563272
 Sr  0.500000    0.500000    0.255129
 Sr  0.500000    0.000000    0.255129
 Sr  0.000000    0.500000    0.255129
 Sr  0.000000    0.000000    0.255129
 Sr  0.997158    0.994234    0.152746
 Sr  0.997303    0.499078    0.152788
 Sr  0.497436    0.993864    0.152791
 Sr  0.497341    0.499463    0.152718
 Ti  0.241796    0.237608    0.003417
```

Ti	0.232222	0.736087	0.999570
Ti	0.741241	0.237977	0.003373
Ti	0.770702	0.735054	0.999437
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Ti	0.250000	0.750000	0.306157
Ti	0.750000	0.250000	0.306157
Ti	0.750000	0.750000	0.306157
Ti	0.250000	0.250000	0.408213
Ti	0.250000	0.750000	0.408213
Ti	0.750000	0.250000	0.408213
Ti	0.750000	0.750000	0.408213
Ti	0.744185	0.742467	0.511106
Ti	0.742844	0.242545	0.509276
Ti	0.244124	0.742513	0.511027
Ti	0.244457	0.242285	0.509267
Ti	0.770702	0.735054	0.612880
Ti	0.741241	0.237977	0.608945
Ti	0.232222	0.736087	0.612747
Ti	0.241796	0.237608	0.608900
Ti	0.750000	0.750000	0.204101
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Ti	0.250000	0.750000	0.204101
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Ti	0.742844	0.242545	0.103042
Ti	0.744185	0.742467	0.101212
C	0.501658	0.759525	0.965227
C	0.501658	0.759525	0.647090
O	0.254871	0.007329	0.002707
O	0.245860	0.507539	0.001269
O	0.750285	0.007641	0.002937
O	0.760750	0.506768	0.000873
O	0.005039	0.252632	0.001663
O	0.001677	0.763749	0.997473
O	0.504944	0.260278	0.000199
O	0.502108	0.754569	0.000566
O	0.250000	0.000000	0.306157
O	0.250000	0.500000	0.306157
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O	0.750000	0.500000	0.306157
O	0.255807	0.256240	0.051441
O	0.250333	0.751737	0.049890
O	0.748558	0.257714	0.051441
O	0.753866	0.749864	0.049848
O	0.000000	0.250000	0.306157

O	0.000000	0.750000	0.306157
O	0.500000	0.250000	0.306157
O	0.500000	0.750000	0.306157
O	0.250000	0.000000	0.408213
O	0.250000	0.500000	0.408213
O	0.750000	0.000000	0.408213
O	0.750000	0.500000	0.408213
O	0.250000	0.250000	0.357185
O	0.250000	0.750000	0.357185
O	0.750000	0.250000	0.357185
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O	0.500000	0.750000	0.408213
O	0.750449	0.752479	0.459490
O	0.752886	0.250720	0.459214
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O	0.250251	0.251457	0.459215
O	0.502993	0.754427	0.511192
O	0.502699	0.252800	0.509516
O	0.002977	0.752986	0.510546
O	0.003071	0.254171	0.510629
O	0.753866	0.749864	0.562470
O	0.748558	0.257714	0.560876
O	0.250333	0.751737	0.562427
O	0.255807	0.256240	0.560877
O	0.752730	0.503180	0.509811
O	0.753942	0.003351	0.510614
O	0.253915	0.503321	0.510090
O	0.252642	0.003288	0.510354
O	0.502108	0.754569	0.611751
O	0.504944	0.260278	0.612119
O	0.001677	0.763749	0.614844
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O	0.760750	0.506768	0.611444
O	0.750285	0.007641	0.609380
O	0.245860	0.507539	0.611049
O	0.254871	0.007329	0.609611
O	0.355419	0.759905	0.951604
O	0.647831	0.759728	0.951526
O	0.647831	0.759728	0.660791
O	0.355419	0.759905	0.660713
O	0.750000	0.750000	0.255129
O	0.750000	0.250000	0.255129
O	0.250000	0.750000	0.255129

O	0.250000	0.250000	0.255129
O	0.500000	0.750000	0.204101
O	0.500000	0.250000	0.204101
O	0.000000	0.750000	0.204101
O	0.000000	0.250000	0.204101
O	0.750000	0.500000	0.204101
O	0.750000	0.000000	0.204101
O	0.250000	0.500000	0.204101
O	0.250000	0.000000	0.204101
O	0.252642	0.003288	0.101964
O	0.253915	0.503321	0.102228
O	0.753942	0.003351	0.101704
O	0.752730	0.503180	0.102507
O	0.003071	0.254171	0.101689
O	0.002977	0.752986	0.101772
O	0.502699	0.252800	0.102802
O	0.502993	0.754427	0.101126
O	0.250251	0.251457	0.153102
O	0.252213	0.751875	0.152837
O	0.752886	0.250720	0.153103
O	0.750449	0.752479	0.152827

Most stable CO_2 adsorption configuration on SrO-terminated $SrTiO_3$(001) surface, as illustrated in Fig. 2a.

```
_chemical_name_common              'Sr28 Ti24 C2 O80'
_cell_length_a                     7.88820
_cell_length_b                     7.88820
_cell_length_c                     38.64670
_cell_angle_alpha                  90
_cell_angle_beta                   90
_cell_angle_gamma                  90
_space_group_name_H-M_alt          'P 1'

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
 Sr  0.000000   0.000000   0.4082130
 Sr  0.000000   0.500000   0.4082130
 Sr  0.500000   0.000000   0.4082130
 Sr  0.500000   0.500000   0.4082130
 Sr  0.000000   0.000000   0.3061570
 Sr  0.000000   0.500000   0.3061570
 Sr  0.500000   0.000000   0.3061570
 Sr  0.500000   0.500000   0.3061570
 Sr  0.010784   0.011726   0.0033600
 Sr  0.999082   0.506977   0.0011180
 Sr  0.506349   0.000678   0.0010620
 Sr  0.487067   0.489235   0.9992690
 Sr  0.487067   0.489235   0.6130480
 Sr  0.506349   0.000678   0.6112560
 Sr  0.999082   0.506977   0.6112000
 Sr  0.010784   0.011726   0.6089580
 Sr  0.494203   0.494377   0.5098570
 Sr  0.497871   0.008432   0.5099880
 Sr  0.008262   0.498142   0.5099120
 Sr  0.007404   0.007758   0.5099670
 Sr  0.500000   0.500000   0.2041010
 Sr  0.500000   0.000000   0.2041010
 Sr  0.000000   0.500000   0.2041010
 Sr  0.000000   0.000000   0.2041010
 Sr  0.007404   0.007758   0.1023510
```

Sr	0.008262	0.498142	0.1024060
Sr	0.497871	0.008432	0.1023300
Sr	0.494203	0.494377	0.1024610
Ti	0.250000	0.250000	0.3571850
Ti	0.250000	0.750000	0.3571850
Ti	0.750000	0.250000	0.3571850
Ti	0.750000	0.750000	0.3571850
Ti	0.252587	0.253451	0.0484100
Ti	0.253884	0.751021	0.0470410
Ti	0.750162	0.254628	0.0470140
Ti	0.751632	0.751993	0.0547790
Ti	0.751632	0.751993	0.5575380
Ti	0.750162	0.254628	0.5653040
Ti	0.253884	0.751021	0.5652770
Ti	0.252587	0.253451	0.5639070
Ti	0.752053	0.752274	0.4577630
Ti	0.752911	0.255830	0.4605020
Ti	0.255645	0.753148	0.4604970
Ti	0.251662	0.251873	0.4593760
Ti	0.750000	0.750000	0.2551290
Ti	0.750000	0.250000	0.2551290
Ti	0.250000	0.750000	0.2551290
Ti	0.250000	0.250000	0.2551290
Ti	0.251662	0.251873	0.1529410
Ti	0.255645	0.753148	0.1518200
Ti	0.752911	0.255830	0.1518150
Ti	0.752053	0.752274	0.1545540
C	0.706921	0.707332	0.966475
C	0.706921	0.707332	0.645843
O	0.250000	0.000000	0.357185
O	0.250000	0.500000	0.357185
O	0.750000	0.000000	0.357185
O	0.750000	0.500000	0.357185
O	0.250000	0.250000	0.408213
O	0.250000	0.750000	0.408213
O	0.750000	0.250000	0.408213
O	0.750000	0.750000	0.408213
O	0.000000	0.250000	0.357185
O	0.000000	0.750000	0.357185
O	0.500000	0.250000	0.357185
O	0.500000	0.750000	0.357185
O	0.249219	0.999519	0.049875
O	0.253835	0.499771	0.051332
O	0.749698	0.994025	0.052967
O	0.746278	0.504570	0.043052
O	0.250000	0.250000	0.306157

O	0.250000	0.750000	0.306157
O	0.750000	0.250000	0.306157
O	0.750000	0.750000	0.306157
O	0.999674	0.252807	0.049863
O	0.994098	0.745570	0.052907
O	0.499940	0.250030	0.051287
O	0.504558	0.749892	0.043175
O	0.253421	0.253325	0.999066
O	0.221377	0.745079	0.000125
O	0.746125	0.220896	0.000124
O	0.801212	0.800763	0.987780
O	0.801212	0.800763	0.624537
O	0.746125	0.220896	0.612193
O	0.221377	0.745079	0.612192
O	0.253421	0.253325	0.613252
O	0.504558	0.749892	0.569142
O	0.499940	0.250030	0.561030
O	0.994098	0.745570	0.559410
O	0.999674	0.252807	0.562454
O	0.730241	0.730134	0.511204
O	0.752202	0.263162	0.510363
O	0.263012	0.752161	0.510347
O	0.246553	0.246361	0.510110
O	0.746278	0.504570	0.569265
O	0.749698	0.994025	0.559350
O	0.253835	0.499771	0.560986
O	0.249219	0.999519	0.562443
O	0.499959	0.747674	0.457984
O	0.498766	0.248441	0.459675
O	0.996133	0.749065	0.461396
O	0.998773	0.246700	0.458908
O	0.749559	0.499869	0.457982
O	0.747621	0.996028	0.461411
O	0.247067	0.498610	0.459678
O	0.248487	0.998661	0.458893
O	0.759086	0.557831	0.958396
O	0.557898	0.760735	0.958385
O	0.557898	0.760735	0.653933
O	0.759086	0.557831	0.653921
O	0.750000	0.750000	0.204101
O	0.750000	0.250000	0.204101
O	0.250000	0.750000	0.204101
O	0.250000	0.250000	0.204101
O	0.500000	0.750000	0.255129
O	0.500000	0.250000	0.255129
O	0.000000	0.750000	0.255129

O	0.000000	0.250000	0.255129
O	0.750000	0.500000	0.255129
O	0.750000	0.000000	0.255129
O	0.250000	0.500000	0.255129
O	0.250000	0.000000	0.255129
O	0.248487	0.998661	0.153424
O	0.247067	0.498610	0.152639
O	0.747621	0.996028	0.150906
O	0.749559	0.499869	0.154335
O	0.998773	0.246700	0.153409
O	0.996133	0.749065	0.150921
O	0.498766	0.248441	0.152642
O	0.499959	0.747674	0.154333
O	0.246553	0.246361	0.102208
O	0.263012	0.752161	0.101971
O	0.752202	0.263162	0.101955
O	0.730241	0.730134	0.101114

CO_2 adsorption configuration on SrO-terminated $SrTiO_3$(001) surface, as illustrated in Fig. S7a.

```
_chemical_name_common                  'Sr28 Ti24 C2 O80'
_cell_length_a                         7.88820
_cell_length_b                         7.88820
_cell_length_c                         38.64670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_type_symbol
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
 Sr  0.490931     0.506313     0.997930
 Sr  0.490889     0.507466     0.614259
 Sr  0.490012     0.497397     0.509999
 Sr  0.006610     0.507053     0.998033
 Sr  0.006762     0.507421     0.614255
 Sr  0.007344     0.497204     0.510027
 Sr  0.494137     0.009691     0.001783
 Sr  0.493573     0.010400     0.610407
 Sr  0.492829     0.011418     0.510407
 Sr  0.005606     0.010006     0.001902
 Sr  0.005236     0.010698     0.610360
 Sr  0.004296     0.011882     0.510452
 Sr  0.491857     0.496557     0.102241
 Sr  0.009213     0.497255     0.102258
 Sr  0.494907     0.011393     0.101833
 Sr  0.006471     0.011040     0.101887
 Sr  0.499995     0.499995     0.408208
 Sr  0.499995     0.499995     0.306160
 Sr  0.000005     0.499995     0.408208
 Sr  0.000005     0.499995     0.306160
 Sr  0.499995     0.000005     0.408208
 Sr  0.499995     0.000005     0.306160
 Sr  0.000005     0.000005     0.408208
 Sr  0.000005     0.000005     0.306160
 Sr  0.000005     0.000005     0.204104
 Sr  0.499995     0.000005     0.204104
```

Sr	0.000005	0.499995	0.204104
Sr	0.499995	0.499995	0.204104
Ti	0.249774	0.258066	0.047710
Ti	0.249054	0.258725	0.564512
Ti	0.248485	0.253188	0.459463
Ti	0.749767	0.750284	0.055515
Ti	0.749188	0.750685	0.556733
Ti	0.746957	0.754201	0.457451
Ti	0.250017	0.752805	0.046882
Ti	0.749657	0.258170	0.045623
Ti	0.748990	0.258764	0.566575
Ti	0.248987	0.753456	0.565377
Ti	0.748602	0.257308	0.460801
Ti	0.246778	0.754833	0.460519
Ti	0.250861	0.252953	0.152830
Ti	0.752402	0.754088	0.154853
Ti	0.252942	0.754532	0.151783
Ti	0.750934	0.256973	0.151476
Ti	0.250005	0.250005	0.357184
Ti	0.750000	0.750000	0.357184
Ti	0.250005	0.750000	0.357184
Ti	0.750000	0.250005	0.357184
Ti	0.750000	0.250005	0.255129
Ti	0.250005	0.750000	0.255129
Ti	0.750000	0.750000	0.255129
Ti	0.250005	0.250005	0.255129
C	0.748240	0.703672	0.649880
C	0.747347	0.702997	0.962330
O	0.249799	0.255484	0.998622
O	0.249770	0.255974	0.613603
O	0.249820	0.245844	0.510136
O	0.500339	0.249801	0.050329
O	0.500516	0.250754	0.561892
O	0.500662	0.247824	0.459494
O	0.998873	0.251410	0.050246
O	0.999099	0.251855	0.561963
O	0.000504	0.246672	0.459425
O	0.250595	0.499043	0.051792
O	0.250366	0.499680	0.560459
O	0.250292	0.498157	0.459732
O	0.248918	0.999161	0.049383
O	0.249229	0.999720	0.562854
O	0.251446	0.998486	0.458954
O	0.750254	0.987819	0.049656
O	0.748572	0.506138	0.041388
O	0.993486	0.745613	0.047872

O	0.505496	0.747472	0.047291
O	0.505941	0.747866	0.564905
O	0.993781	0.746612	0.564558
O	0.749327	0.729744	0.510749
O	0.749343	0.506656	0.570984
O	0.750550	0.988471	0.562252
O	0.502623	0.747016	0.459524
O	0.751708	0.498936	0.458310
O	0.999273	0.748181	0.459770
O	0.750428	0.995331	0.461201
O	0.247984	0.739921	0.999804
O	0.749487	0.218086	0.999467
O	0.749676	0.217710	0.612705
O	0.248970	0.740552	0.612461
O	0.750449	0.258767	0.510802
O	0.251268	0.751982	0.510352
O	0.748915	0.540073	0.653931
O	0.749008	0.539402	0.958275
O	0.891851	0.782491	0.645925
O	0.890409	0.782564	0.966464
O	0.604037	0.781835	0.646500
O	0.602614	0.780370	0.965545
O	0.249424	0.245525	0.102138
O	0.499270	0.247359	0.152822
O	0.999128	0.246605	0.152849
O	0.248463	0.497905	0.152572
O	0.249200	0.998239	0.153324
O	0.749521	0.257482	0.101462
O	0.749167	0.498714	0.153839
O	0.500472	0.746901	0.152769
O	0.747940	0.730754	0.101524
O	0.997081	0.747675	0.152587
O	0.748401	0.995155	0.151191
O	0.249883	0.751525	0.101945
O	0.250005	0.250005	0.408208
O	0.250005	0.250005	0.306160
O	0.499995	0.250005	0.357184
O	0.000005	0.250005	0.357184
O	0.250005	0.499995	0.357184
O	0.250005	0.000005	0.357184
O	0.750000	0.499995	0.357184
O	0.750000	0.750000	0.408208
O	0.499995	0.750000	0.357184
O	0.750000	0.750000	0.306160
O	0.000005	0.750000	0.357184
O	0.750000	0.000005	0.357184

O	0.250005	0.750000	0.408208
O	0.750000	0.250005	0.408208
O	0.250005	0.750000	0.306160
O	0.750000	0.250005	0.306160
O	0.750000	0.250005	0.204104
O	0.250005	0.750000	0.204104
O	0.750000	0.000005	0.255129
O	0.000005	0.750000	0.255129
O	0.750000	0.750000	0.204104
O	0.499995	0.750000	0.255129
O	0.750000	0.499995	0.255129
O	0.250005	0.000005	0.255129
O	0.250005	0.499995	0.255129
O	0.000005	0.250005	0.255129
O	0.499995	0.250005	0.255129
O	0.250005	0.250005	0.204104

CO_2 adsorption configuration on SrO-terminated $SrTiO_3$(001) surface, as illustrated in Fig. S7b.

```
_chemical_name_common                  'Sr28 Ti24 C2 O80'
_cell_length_a                         7.88820
_cell_length_b                         7.88820
_cell_length_c                         38.64670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
 Sr  0.000000   0.000000   0.408214
 Sr  0.000000   0.500000   0.408214
 Sr  0.500000   0.000000   0.408214
 Sr  0.500000   0.500000   0.408214
 Sr  0.000000   0.000000   0.306159
 Sr  0.000000   0.500000   0.306159
 Sr  0.500000   0.000000   0.306159
 Sr  0.500000   0.500000   0.306159
 Sr  0.006972   0.997554   0.002133
 Sr  0.006972   0.502446   0.002133
 Sr  0.490068   0.995797   0.001527
 Sr  0.490068   0.504203   0.001527
 Sr  0.490073   0.504185   0.610787
 Sr  0.490073   0.995815   0.610787
 Sr  0.006938   0.502438   0.610174
 Sr  0.006938   0.997562   0.610174
 Sr  0.494897   0.494091   0.509757
 Sr  0.494897   0.005909   0.509757
 Sr  0.000843   0.494153   0.509826
 Sr  0.000843   0.005847   0.509826
 Sr  0.500000   0.500000   0.204103
 Sr  0.500000   0.000000   0.204103
 Sr  0.000000   0.500000   0.204103
 Sr  0.000000   0.000000   0.204103
 Sr  0.000839   0.005866   0.102483
 Sr  0.000839   0.494134   0.102483
```

Sr	0.494898	0.005918	0.102550
Sr	0.494898	0.494082	0.102550
Ti	0.250000	0.250000	0.357186
Ti	0.250000	0.750000	0.357186
Ti	0.750000	0.250000	0.357186
Ti	0.750000	0.750000	0.357186
Ti	0.249319	0.250000	0.048134
Ti	0.245003	0.750000	0.048960
Ti	0.747771	0.250000	0.046235
Ti	0.746656	0.750000	0.053849
Ti	0.746650	0.750000	0.558468
Ti	0.747734	0.250000	0.566070
Ti	0.245010	0.750000	0.563361
Ti	0.249306	0.250000	0.564169
Ti	0.744854	0.750000	0.457872
Ti	0.748369	0.250000	0.460500
Ti	0.247283	0.750000	0.460149
Ti	0.247367	0.250000	0.459534
Ti	0.750000	0.750000	0.255131
Ti	0.750000	0.250000	0.255131
Ti	0.250000	0.750000	0.255131
Ti	0.250000	0.250000	0.255131
Ti	0.247373	0.250000	0.152778
Ti	0.247250	0.750000	0.152157
Ti	0.748377	0.250000	0.151808
Ti	0.744822	0.750000	0.154436
C	0.742934	0.750000	0.963407
C	0.742900	0.750000	0.648919
O	0.250000	0.000000	0.357186
O	0.250000	0.500000	0.357186
O	0.750000	0.000000	0.357186
O	0.750000	0.500000	0.357186
O	0.250000	0.250000	0.408214
O	0.250000	0.750000	0.408214
O	0.750000	0.250000	0.408214
O	0.750000	0.750000	0.408214
O	0.000000	0.250000	0.357186
O	0.000000	0.750000	0.357186
O	0.500000	0.250000	0.357186
O	0.500000	0.750000	0.357186
O	0.251646	1.000291	0.050327
O	0.251646	0.499709	0.050327
O	0.751435	0.997204	0.048439
O	0.751435	0.502796	0.048439
O	0.250000	0.250000	0.306159
O	0.250000	0.750000	0.306159

O	0.750000	0.250000	0.306159
O	0.750000	0.750000	0.306159
O	0.000751	0.250000	0.049218
O	0.999350	0.750000	0.054193
O	0.501209	0.250000	0.050733
O	0.504544	0.750000	0.045652
O	0.253929	0.250000	0.998947
O	0.229777	0.750000	0.000842
O	0.747239	0.250000	0.998354
O	0.796138	0.750000	0.997320
O	0.579522	0.750000	0.959437
O	0.856222	0.750000	0.940718
O	0.856199	0.750000	0.671608
O	0.579485	0.750000	0.652889
O	0.796097	0.750000	0.615006
O	0.747206	0.250000	0.613953
O	0.229730	0.750000	0.611474
O	0.253956	0.250000	0.613356
O	0.504518	0.750000	0.566673
O	0.501190	0.250000	0.561572
O	0.999319	0.750000	0.558122
O	0.000734	0.250000	0.563084
O	0.734189	0.750000	0.511165
O	0.753946	0.250000	0.510262
O	0.266193	0.750000	0.510114
O	0.247695	0.250000	0.510251
O	0.751402	0.502793	0.563877
O	0.751402	0.997207	0.563877
O	0.251626	0.499717	0.561980
O	0.251626	1.000283	0.561980
O	0.502672	0.750000	0.457888
O	0.500946	0.250000	0.459669
O	0.000133	0.750000	0.461196
O	0.001017	0.250000	0.458899
O	0.751811	0.501714	0.459697
O	0.751811	-0.001714	0.459697
O	0.250922	0.500068	0.459322
O	0.250922	-0.000068	0.459322
O	0.750000	0.750000	0.204103
O	0.750000	0.250000	0.204103
O	0.250000	0.750000	0.204103
O	0.250000	0.250000	0.204103
O	0.500000	0.750000	0.255131
O	0.500000	0.250000	0.255131
O	0.000000	0.750000	0.255131
O	0.000000	0.250000	0.255131

O	0.750000	0.500000	0.255131
O	0.750000	0.000000	0.255131
O	0.250000	0.500000	0.255131
O	0.250000	0.000000	0.255131
O	0.250958	-0.000070	0.152988
O	0.250958	0.500070	0.152988
O	0.751849	-0.001717	0.152615
O	0.751849	0.501717	0.152615
O	0.001038	0.250000	0.153419
O	0.000169	0.750000	0.151103
O	0.500970	0.250000	0.152634
O	0.502689	0.750000	0.154422
O	0.247667	0.250000	0.102059
O	0.266227	0.750000	0.102191
O	0.754011	0.250000	0.102047
O	0.734210	0.750000	0.101152

CO_2 adsorption configuration on SrO-terminated $SrTiO_3$(001) surface, as illustrated in Fig. S7c.

```
_chemical_name_common                  'Sr28 Ti24 C2 O80'
_cell_length_a                         7.88820
_cell_length_b                         7.88820
_cell_length_c                         38.64670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_type_symbol
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
 Sr  0.000000     0.000000     0.408214
 Sr  0.000000     0.500000     0.408214
 Sr  0.500000     0.000000     0.408214
 Sr  0.500000     0.500000     0.408214
 Sr  0.000000     0.000000     0.306159
 Sr  0.000000     0.500000     0.306159
 Sr  0.500000     0.000000     0.306159
 Sr  0.500000     0.500000     0.306159
 Sr -0.002230    -0.002230     0.000080
 Sr  0.004021     0.496354     0.003951
 Sr  0.496354     0.004021     0.003951
 Sr  0.502575     0.502575     0.000024
 Sr  0.502571     0.502571     0.612283
 Sr  0.496351     0.004026     0.608357
 Sr  0.004026     0.496351     0.608357
 Sr -0.002235    -0.002235     0.612230
 Sr  0.495485     0.495485     0.509980
 Sr  0.495693     0.004483     0.509483
 Sr  0.004483     0.495693     0.509483
 Sr  0.004691     0.004691     0.509979
 Sr  0.500000     0.500000     0.204103
 Sr  0.500000     0.000000     0.204103
 Sr  0.000000     0.500000     0.204103
 Sr  0.000000     0.000000     0.204103
 Sr  0.004699     0.004699     0.102332
 Sr  0.004489     0.495689     0.102828
```

Sr	0.495689	0.004489	0.102828
Sr	0.495481	0.495481	0.102330
Ti	0.250000	0.250000	0.357186
Ti	0.250000	0.750000	0.357186
Ti	0.750000	0.250000	0.357186
Ti	0.750000	0.750000	0.357186
Ti	0.250169	0.250169	0.048031
Ti	0.250197	0.750134	0.047749
Ti	0.750134	0.250197	0.047749
Ti	0.750152	0.750152	0.054036
Ti	0.750149	0.750149	0.558273
Ti	0.750135	0.250192	0.564554
Ti	0.250192	0.750135	0.564554
Ti	0.250166	0.250166	0.564273
Ti	0.750072	0.750072	0.457767
Ti	0.750077	0.250069	0.460250
Ti	0.250069	0.750077	0.460250
Ti	0.250071	0.250071	0.459567
Ti	0.750000	0.750000	0.255131
Ti	0.750000	0.250000	0.255131
Ti	0.250000	0.750000	0.255131
Ti	0.250000	0.250000	0.255131
Ti	0.250073	0.250073	0.152748
Ti	0.250070	0.750078	0.152057
Ti	0.750078	0.250070	0.152057
Ti	0.750075	0.750075	0.154545
C	0.750101	0.750101	0.961298
C	0.750110	0.750110	0.651018
O	0.250000	0.000000	0.357186
O	0.250000	0.500000	0.357186
O	0.750000	0.000000	0.357186
O	0.750000	0.500000	0.357186
O	0.250000	0.250000	0.408214
O	0.250000	0.750000	0.408214
O	0.750000	0.250000	0.408214
O	0.750000	0.750000	0.408214
O	0.000000	0.250000	0.357186
O	0.000000	0.750000	0.357186
O	0.500000	0.250000	0.357186
O	0.500000	0.750000	0.357186
O	0.251390	1.000047	0.050339
O	0.248624	0.499959	0.050373
O	0.749451	0.997653	0.049305
O	0.750587	0.502395	0.049339
O	0.250000	0.250000	0.306159
O	0.250000	0.750000	0.306159

O	0.750000	0.250000	0.306159
O	0.750000	0.750000	0.306159
O	1.000047	0.251390	0.050339
O	0.997653	0.749451	0.049305
O	0.499959	0.248624	0.050373
O	0.502395	0.750587	0.049339
O	0.250060	0.250060	0.999140
O	0.250099	0.749847	-0.000397
O	0.749847	0.250099	-0.000397
O	0.749826	0.749826	0.997135
O	0.853192	0.853192	0.947269
O	0.647234	0.647234	0.947149
O	0.647220	0.647220	0.665161
O	0.853183	0.853183	0.665052
O	0.749856	0.749856	0.615180
O	0.749847	0.250084	0.612701
O	0.250084	0.749847	0.612701
O	0.250064	0.250064	0.613164
O	0.502403	0.750590	0.562969
O	0.499961	0.248626	0.561933
O	0.997649	0.749451	0.562996
O	1.000049	0.251393	0.561967
O	0.750087	0.750087	0.511095
O	0.750025	0.249958	0.510161
O	0.249958	0.750025	0.510161
O	0.249952	0.249952	0.510058
O	0.750590	0.502403	0.562969
O	0.749451	0.997649	0.562996
O	0.248626	0.499961	0.561933
O	0.251393	1.000049	0.561967
O	0.501607	0.750022	0.459598
O	0.500097	0.249974	0.459244
O	-0.001613	0.749951	0.459584
O	-0.000117	0.250018	0.459237
O	0.750022	0.501607	0.459598
O	0.749951	-0.001613	0.459584
O	0.249974	0.500097	0.459244
O	0.250018	-0.000117	0.459237
O	0.750000	0.750000	0.204103
O	0.750000	0.250000	0.204103
O	0.250000	0.750000	0.204103
O	0.250000	0.250000	0.204103
O	0.500000	0.750000	0.255131
O	0.500000	0.250000	0.255131
O	0.000000	0.750000	0.255131
O	0.000000	0.250000	0.255131

O	0.750000	0.500000	0.255131
O	0.750000	0.000000	0.255131
O	0.250000	0.500000	0.255131
O	0.250000	0.000000	0.255131
O	0.250018	-0.000118	0.153077
O	0.249974	0.500097	0.153070
O	0.749949	-0.001618	0.152728
O	0.750021	0.501611	0.152712
O	-0.000118	0.250018	0.153077
O	-0.001618	0.749949	0.152728
O	0.500097	0.249974	0.153070
O	0.501611	0.750021	0.152712
O	0.249952	0.249952	0.102254
O	0.249946	0.750022	0.102150
O	0.750022	0.249946	0.102150
O	0.750100	0.750100	0.101212

CO_2 adsorption configuration on SrO-terminated $SrTiO_3$(001) surface, as illustrated in Fig. S7d.

```
_chemical_name_common                  'Sr28 Ti24 C2 O80'
_cell_length_a                         7.88820
_cell_length_b                         7.88820
_cell_length_c                         38.64670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_type_symbol
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
 Sr  0.000000   0.000000   0.408214
 Sr  0.000000   0.500000   0.408214
 Sr  0.500000   0.000000   0.408214
 Sr  0.500000   0.500000   0.408214
 Sr  0.000000   0.000000   0.306159
 Sr  0.000000   0.500000   0.306159
 Sr  0.500000   0.000000   0.306159
 Sr  0.500000   0.500000   0.306159
 Sr  0.006816   0.991668   0.001736
 Sr  0.006816   0.508332   0.001736
 Sr  0.493184   0.991668   0.001736
 Sr  0.493184   0.508332   0.001736
 Sr  0.493187   0.508322   0.610572
 Sr  0.493187   0.991678   0.610572
 Sr  0.006813   0.508322   0.610572
 Sr  0.006813   0.991678   0.610572
 Sr  0.496563   0.493597   0.509805
 Sr  0.496563   0.006403   0.509805
 Sr  0.003437   0.493597   0.509805
 Sr  0.003437   0.006403   0.509805
 Sr  0.500000   0.500000   0.204103
 Sr  0.500000   0.000000   0.204103
 Sr  0.000000   0.500000   0.204103
 Sr  0.000000   0.000000   0.204103
 Sr  0.003441   0.006408   0.102504
 Sr  0.003441   0.493592   0.102504
```

Sr	0.496559	0.006408	0.102504
Sr	0.496559	0.493592	0.102504
Ti	0.250000	0.250000	0.357186
Ti	0.250000	0.750000	0.357186
Ti	0.750000	0.250000	0.357186
Ti	0.750000	0.750000	0.357186
Ti	0.250000	0.250000	0.047397
Ti	0.250000	0.750000	0.049380
Ti	0.750000	0.250000	0.046033
Ti	0.750000	0.750000	0.054419
Ti	0.750000	0.750000	0.557891
Ti	0.750000	0.250000	0.566273
Ti	0.250000	0.750000	0.562928
Ti	0.250000	0.250000	0.564903
Ti	0.750000	0.750000	0.457715
Ti	0.750000	0.250000	0.460522
Ti	0.250000	0.750000	0.459889
Ti	0.250000	0.250000	0.459678
Ti	0.750000	0.750000	0.255131
Ti	0.750000	0.250000	0.255131
Ti	0.250000	0.750000	0.255131
Ti	0.250000	0.250000	0.255131
Ti	0.250000	0.250000	0.152633
Ti	0.250000	0.750000	0.152421
Ti	0.750000	0.250000	0.151786
Ti	0.750000	0.750000	0.154595
C	0.750000	0.750000	0.963359
C	0.750000	0.750000	0.648966
O	0.250000	0.000000	0.357186
O	0.250000	0.500000	0.357186
O	0.750000	0.000000	0.357186
O	0.750000	0.500000	0.357186
O	0.250000	0.250000	0.408214
O	0.250000	0.750000	0.408214
O	0.750000	0.250000	0.408214
O	0.750000	0.750000	0.408214
O	0.000000	0.250000	0.357186
O	0.000000	0.750000	0.357186
O	0.500000	0.250000	0.357186
O	0.500000	0.750000	0.357186
O	0.250000	1.000493	0.050155
O	0.250000	0.499507	0.050155
O	0.750000	0.997216	0.048751
O	0.750000	0.502784	0.048751
O	0.250000	0.250000	0.306159
O	0.250000	0.750000	0.306159

O	0.750000	0.250000	0.306159
O	0.750000	0.750000	0.306159
O	0.999728	0.250000	0.049698
O	0.998439	0.750000	0.050296
O	0.500272	0.250000	0.049698
O	0.501561	0.750000	0.050296
O	0.250000	0.250000	0.998607
O	0.250000	0.750000	0.000694
O	0.750000	0.250000	0.998224
O	0.750000	0.750000	0.998823
O	0.603290	0.750000	0.949551
O	0.896710	0.750000	0.949551
O	0.896705	0.750000	0.662776
O	0.603295	0.750000	0.662776
O	0.750000	0.750000	0.613498
O	0.750000	0.250000	0.614084
O	0.250000	0.750000	0.611614
O	0.250000	0.250000	0.613694
O	0.501567	0.750000	0.562011
O	0.500274	0.250000	0.562607
O	0.998433	0.750000	0.562011
O	0.999726	0.250000	0.562607
O	0.750000	0.750000	0.510819
O	0.750000	0.250000	0.510228
O	0.250000	0.750000	0.510141
O	0.250000	0.250000	0.510185
O	0.750000	0.502781	0.563558
O	0.750000	0.997219	0.563558
O	0.250000	0.499512	0.562147
O	0.250000	1.000488	0.562147
O	0.501351	0.750000	0.459480
O	0.499929	0.250000	0.459298
O	-0.001351	0.750000	0.459480
O	0.000071	0.250000	0.459298
O	0.750000	0.501653	0.459595
O	0.750000	-0.001653	0.459595
O	0.250000	0.500275	0.459292
O	0.250000	-0.000275	0.459292
O	0.750000	0.750000	0.204103
O	0.750000	0.250000	0.204103
O	0.250000	0.750000	0.204103
O	0.250000	0.250000	0.204103
O	0.500000	0.750000	0.255131
O	0.500000	0.250000	0.255131
O	0.000000	0.750000	0.255131
O	0.000000	0.250000	0.255131

O	0.750000	0.500000	0.255131
O	0.750000	0.000000	0.255131
O	0.250000	0.500000	0.255131
O	0.250000	0.000000	0.255131
O	0.250000	-0.000277	0.153020
O	0.250000	0.500277	0.153020
O	0.750000	-0.001656	0.152715
O	0.750000	0.501656	0.152715
O	0.000070	0.250000	0.153015
O	-0.001352	0.750000	0.152830
O	0.499930	0.250000	0.153015
O	0.501352	0.750000	0.152830
O	0.250000	0.250000	0.102125
O	0.250000	0.750000	0.102167
O	0.750000	0.250000	0.102082
O	0.750000	0.750000	0.101490