Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information:

Suppression of Surfaces States at Cubic Perovskite (001) Surfaces by CO_2 Adsorption

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Table S1. Consolidated properties of the cubic perovskites. Goldschmidt tolerance factors were calculated using ionic radii of 12-fold coordinated A-site cations in +2 state, 6-fold coordinated B-site cation in +4 state, and 6-fold coordinated O^{2-}, as tabulated by Shannon.[1]

Compound	Lattice constant (Å)	PBE band gap (eV)	Goldschmidt tolerance factor
$SrTiO_3$	3.95	1.79	1.002
$SrZrO_3$	4.20	3.22	0.947
$SrHfO_3$	4.14	3.74	0.952
$BaTiO_3$	4.04	1.69	1.062
$BaZrO_3$	4.26	3.04	1.004
$BaHfO_3$	4.21	3.54	1.009

Table S2. Consolidated properties of the clean ABO_3(001) surfaces. Stabilization energies refer to the differences in surface energies for undistorted relaxed surfaces and those with the most stable distortion patterns.

Compound	Termination	PBE band gap (eV)	PBE band gap reduction (eV)	Stabilization energy (meV/Å^2)
$SrTiO_3$	SrO	1.55	0.24	0.0
	TiO_2	1.01	0.78	2.0
$SrZrO_3$	SrO	2.83	0.39	30.7
	ZrO_2	2.81	0.41	12.8
$SrHfO_3$	SrO	2.80	0.94	19.7
	HfO_2	3.26	0.48	6.8
$BaTiO_3$	BaO	1.72	-0.03*	2.2
	TiO_2	0.87	0.82	10.5
$BaZrO_3$	BaO	2.77	0.27	0.9
	ZrO_2	2.44	0.60	0.0
$BaHfO_3$	BaO	2.77	0.77	0.0
	HfO_2	2.83	0.71	0.0

**within the accuracy limit*

Table S3. Consolidated properties of the ABO_3(001) surfaces at Θ=0.25 CO_2 coverage.

Compound	Termination	PBE band gap (eV)	CO_2 adsorption energy (eV)
$SrTiO_3$	SrO	1.83	-1.92
	TiO_2	1.46	-1.24
$SrZrO_3$	SrO	3.28	-2.19
	ZrO_2	3.12	-1.70
$SrHfO_3$	SrO	3.67	-2.10
	HfO_2	3.58	-1.69
$BaTiO_3$	BaO	1.76	-1.82
	TiO_2	1.33	-1.49
$BaZrO_3$	BaO	3.08	-1.97
	ZrO_2	2.76	-1.71
$BaHfO_3$	BaO	3.57	-1.79
	HfO_2	3.15	-1.75

Table S4. Consolidated properties of the ABO_3(001) surfaces at Θ=0.50 CO_2 coverage.

Compound	Termination	PBE band gap (eV)	CO_2 adsorption energy (eV)
$SrTiO_3$	SrO	1.85	-1.47
	TiO_2	1.81	-1.20
$SrZrO_3$	SrO	3.28	-1.95
	ZrO_2	3.26	-1.60
$SrHfO_3$	SrO	3.82	-1.81
	HfO_2	3.80	-1.59
$BaTiO_3$	BaO	1.75	-1.38
	TiO_2	1.73	-1.43
$BaZrO_3$	BaO	3.05	-1.60
	ZrO_2	3.00	-1.62
$BaHfO_3$	BaO	3.54	-1.46
	HfO_2	3.48	-1.65

Table S5. Geometries of the CO_3-like complexes formed upon CO_2 chemisorption on the ABO_3(001) surfaces of cubic perovskites at Θ=0.25.

Compound	Termination	Average C-O bond length (Å)	C-O_S bond length (Å)	O-C-O angle (degree)
$SrTiO_3$	SrO	1.29	1.33	122.2
	TiO_2	1.27	1.37	130.8
$SrZrO_3$	SrO	1.28	1.35	122.2
	ZrO_2	1.27	1.36	130.7
$SrHfO_3$	SrO	1.28	1.35	122.7
	HfO_2	1.27	1.37	131.3
$BaTiO_3$	BaO	1.28	1.34	123.3
	TiO_2	1.27	1.35	130.6
$BaZrO_3$	BaO	1.28	1.35	122.9
	ZrO_2	1.27	1.37	129.2
$BaHfO_3$	BaO	1.28	1.36	123.7
	HfO_2	1.27	1.37	129.9

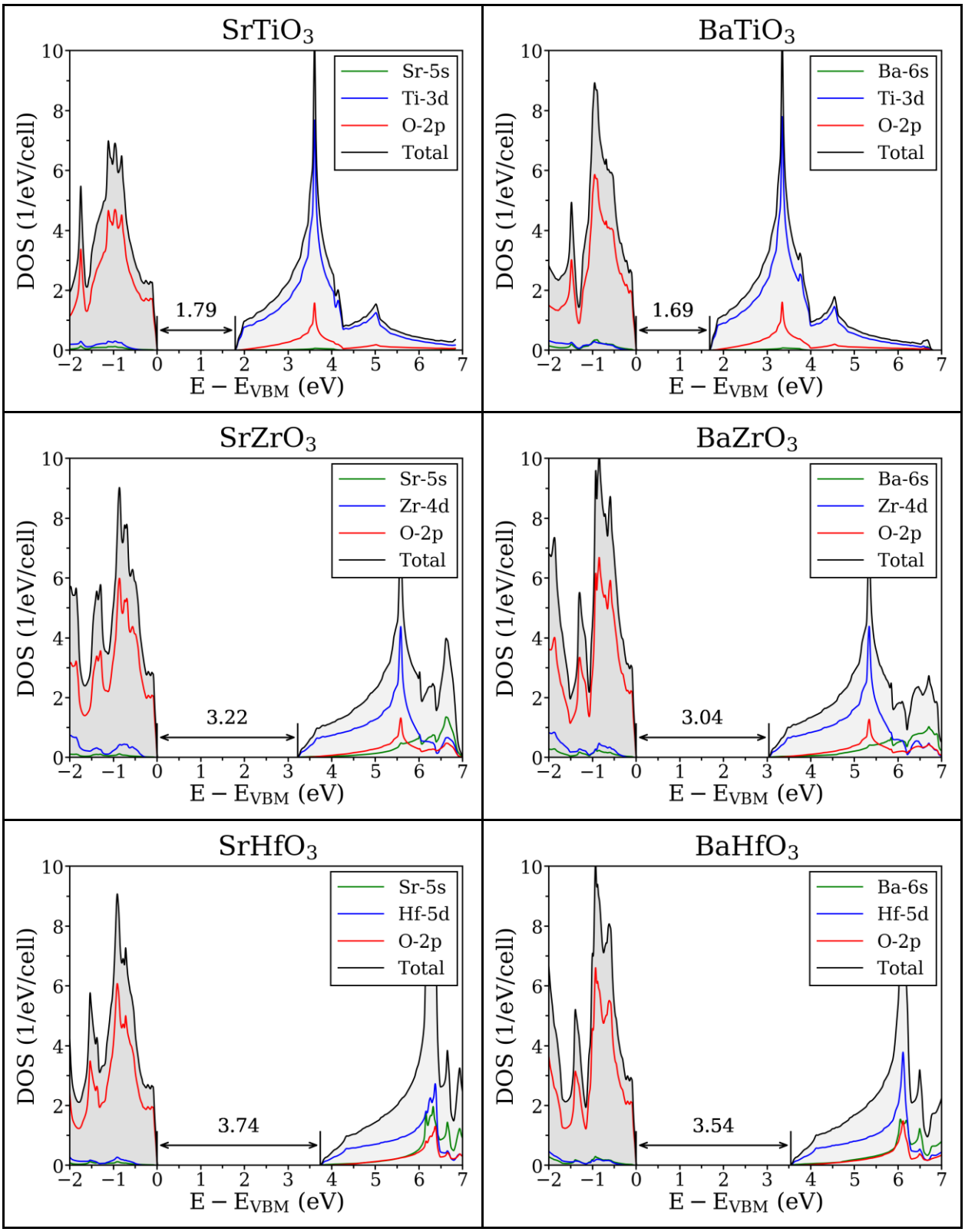

Figure S1. Projected density of states (DOS) for all considered cubic perovskite materials.

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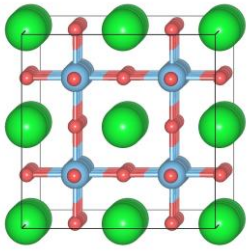
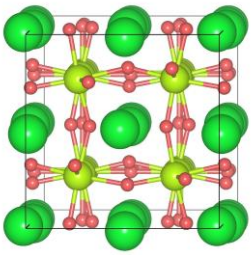
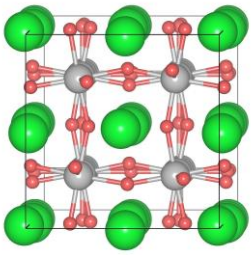
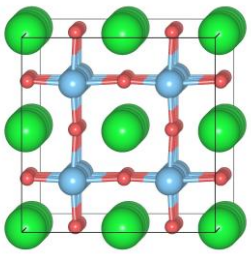
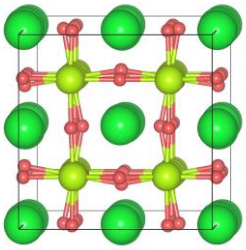
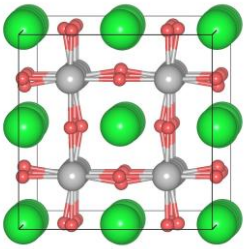
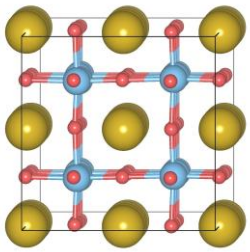
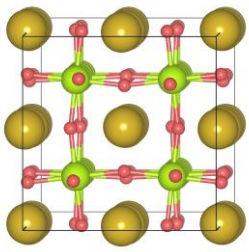
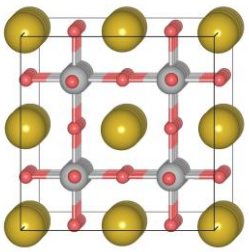
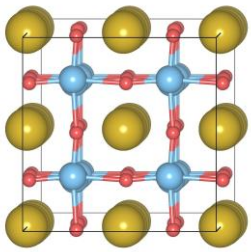
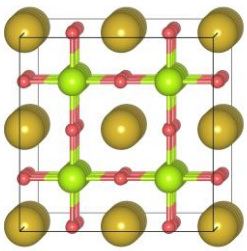
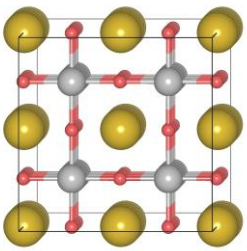
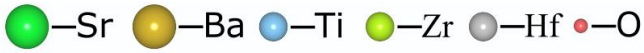
AO-terminated (001)			
BO_2-terminated (001)			
	$BaTiO_3$	$BaZrO_3$	$BaHfO_3$
AO-terminated (001)			
BO_2-terminated (001)			
			

Figure S2. Most stable surface distortion for all considered cubic perovskite surfaces.

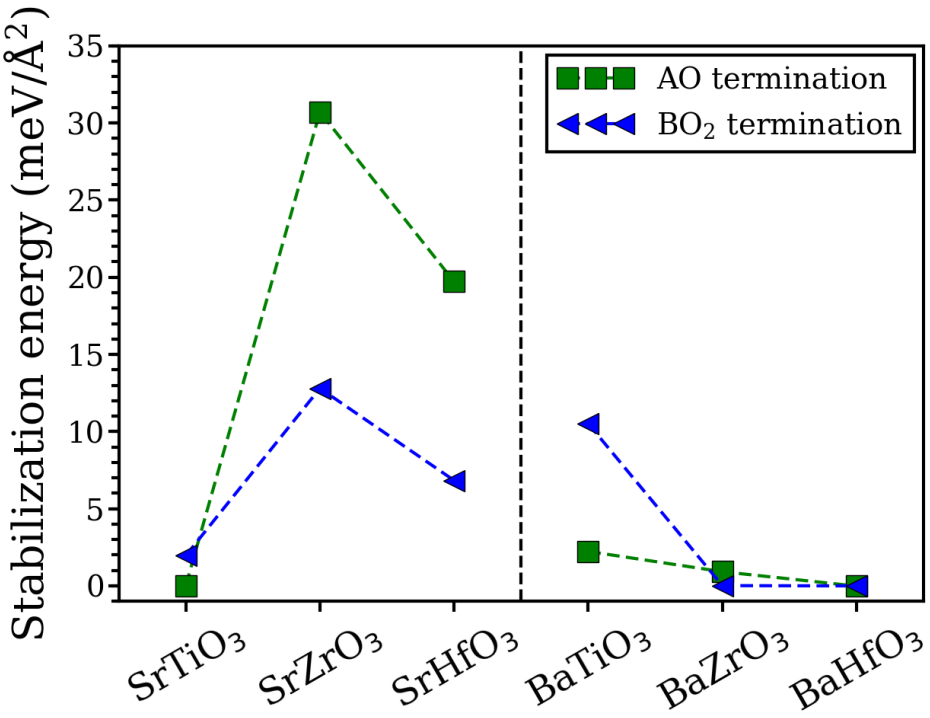


Figure S3. Stabilization energies for different perovskite ABO_3(001) surfaces. Stabilization energies were calculated as differences in surface energies for undistorted relaxed surfaces and those with the most stable distortion patterns. The values are also tabulated in Table S2.

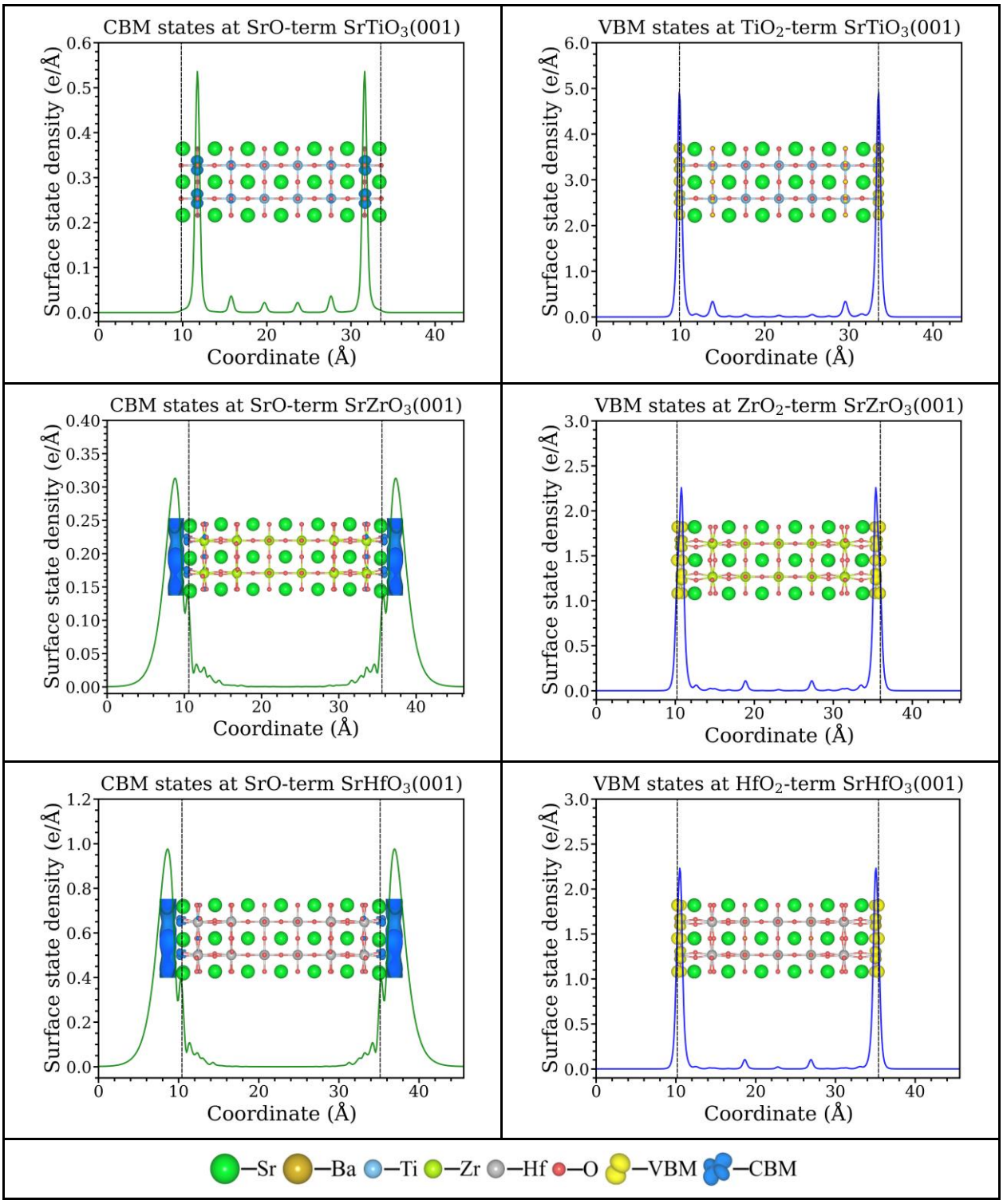


Figure S4. Localization of the surface states at the Sr-containing ABO_3(001). The surface state densities were computed as charge densities for the states within energy limits from the conduction band minima (CBM) or valence band maxima (VBM) levels of the slabs to those of the corresponding bulk compounds.

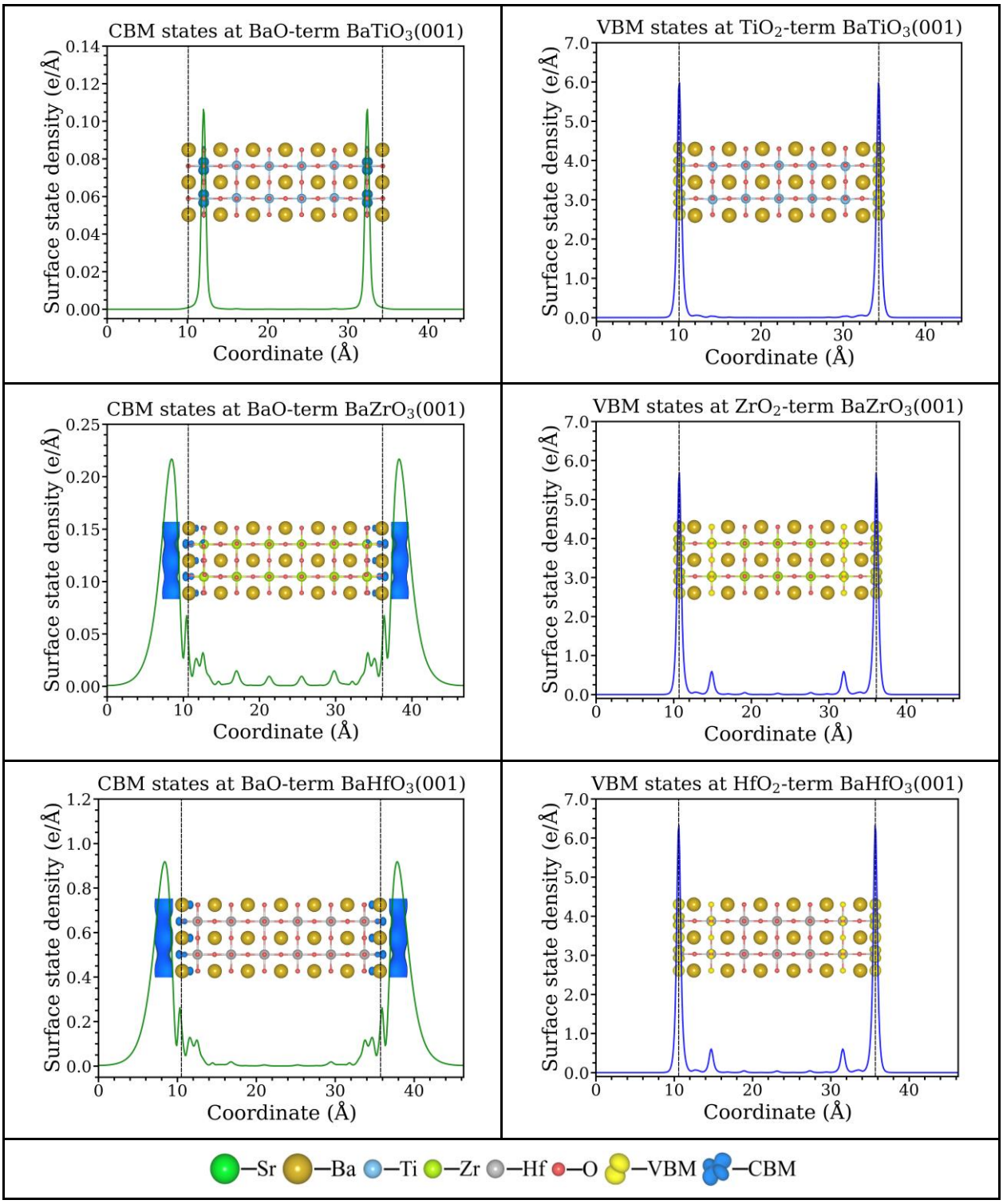


Figure S5. Localization of the surface states at the Ba-containing $ABO_3(001)$. The surface state densities were computed as charge densities for the states within energy limits from the conduction band minima (CBM) or valence band maxima (VBM) levels of the slabs to those of the corresponding bulk compounds.

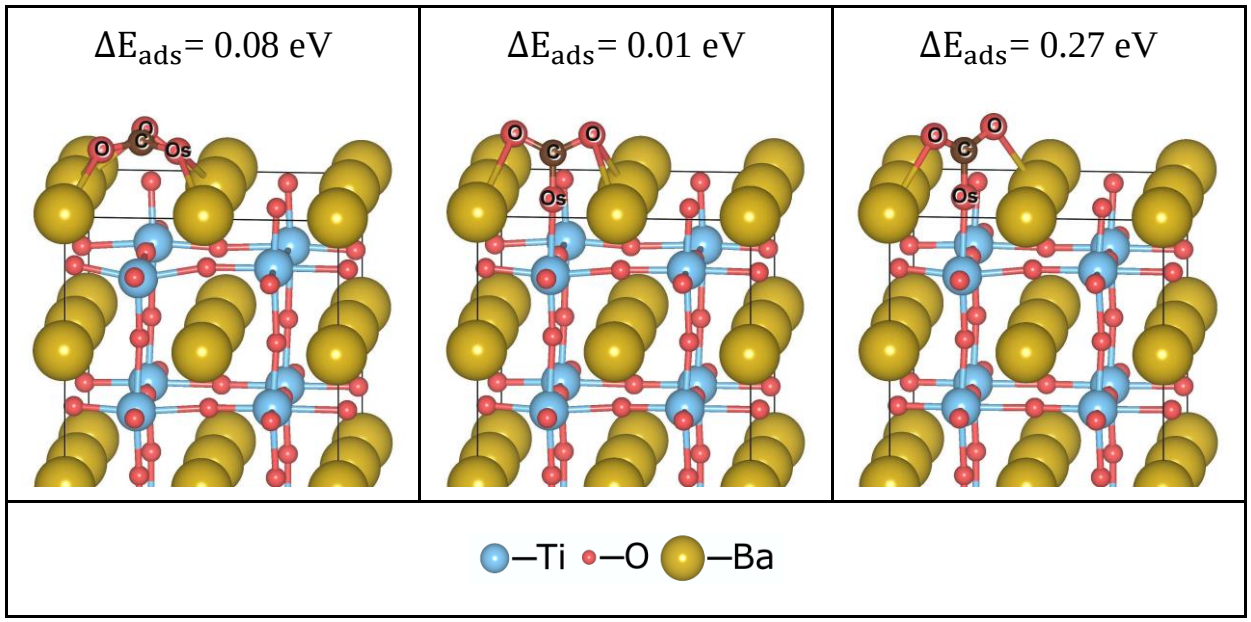


Figure S6. Metastable CO_2 adsorption conformations observed on AO-terminated $BaTiO_3$(001) surface. All systems correspond to Θ=0.25 CO_2 coverage. ΔE_{ads} denotes energy difference between the most stable and specific metastable CO_2 adsorption configuration.

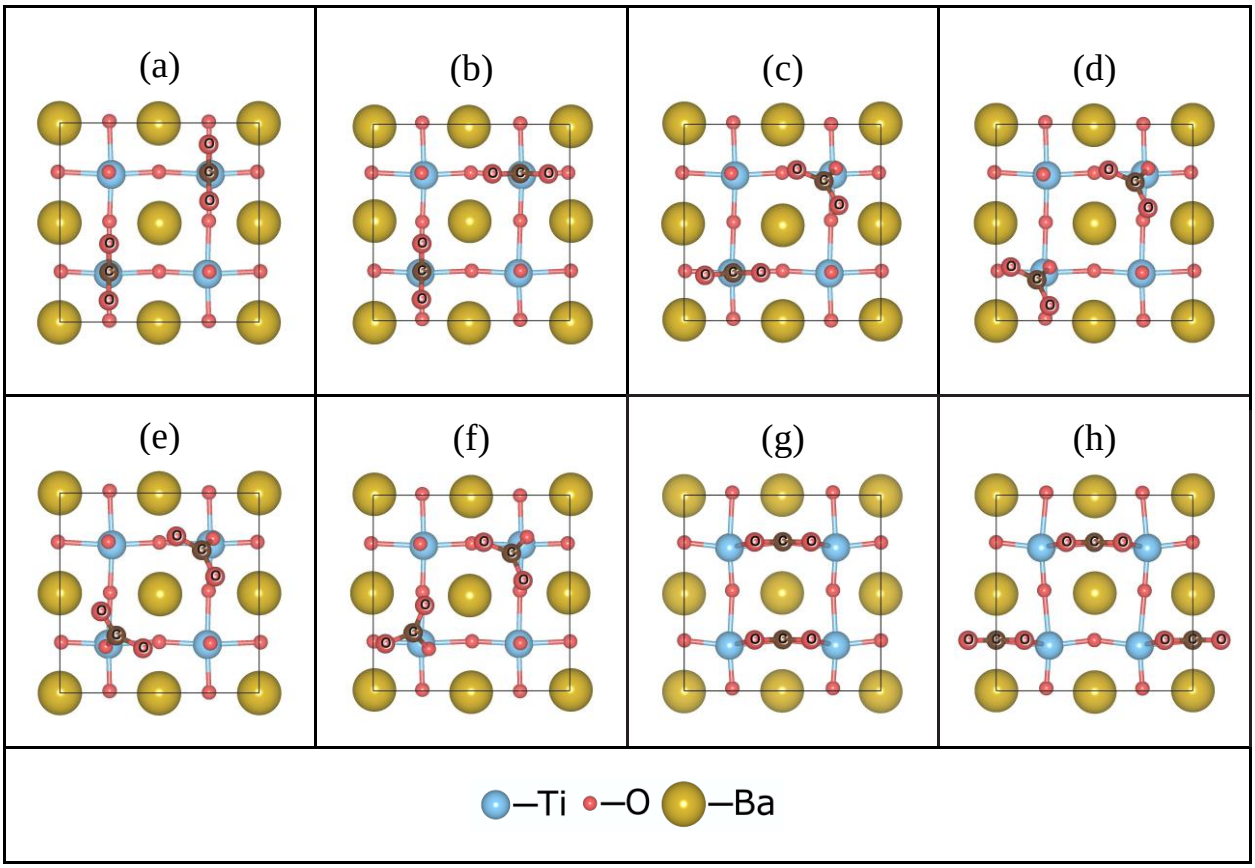


Figure S7. Considered modes for CO_2 adsorption demonstrated for (a-f) BaO- and (g-h) TiO_2-terminated $BaTiO_3$(001) surfaces. All systems correspond to Θ=0.50 CO_2 coverage.

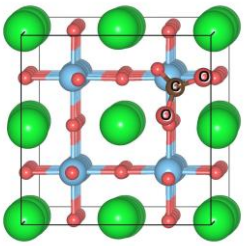
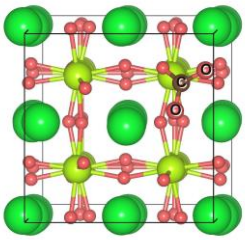
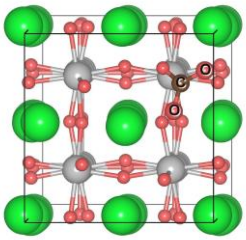
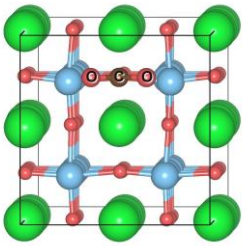
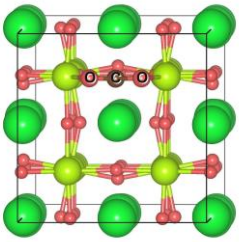
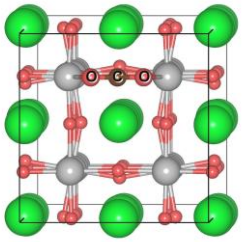
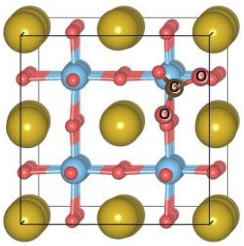
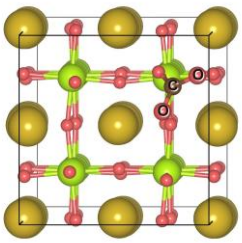
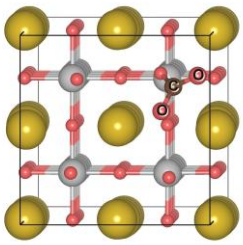
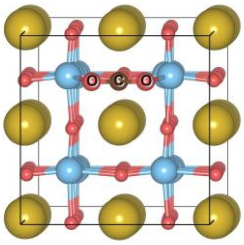
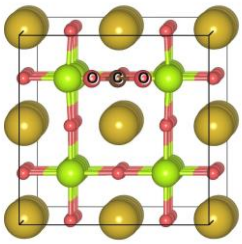
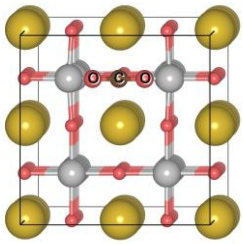
	$SrTiO_3$	$SrZrO_3$	$SrHfO_3$
AO-terminated (001)			
BO_2-terminated (001)			
	$BaTiO_3$	$BaZrO_3$	$BaHfO_3$
AO-terminated (001)			
BO_2-terminated (001)			
			

Figure S8. Surface relaxations of all considered perovskite surfaces upon CO_2 adsorption at Θ=0.25 coverage.

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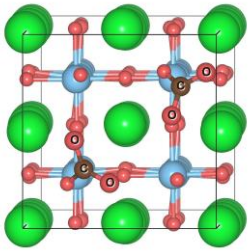
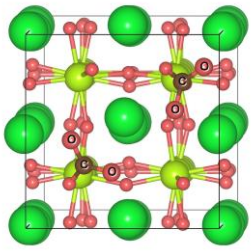
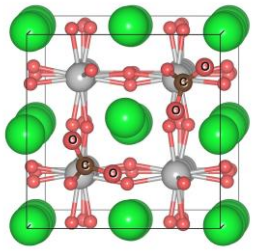
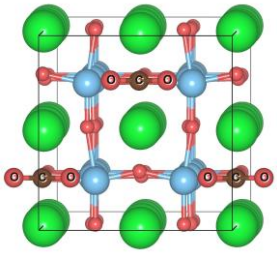
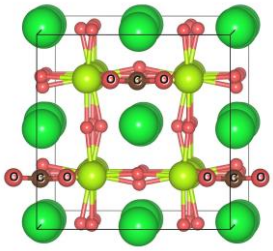
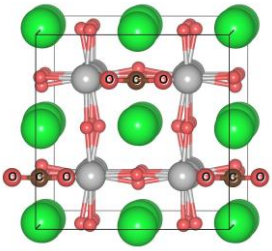
AO-terminated (001)			
BO_2-terminated (001)			
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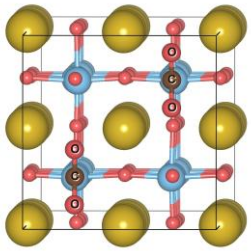
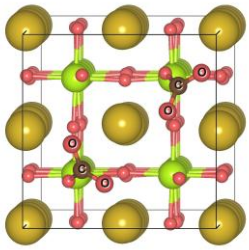
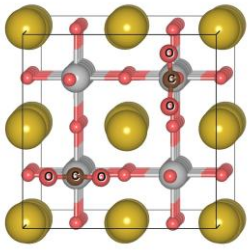
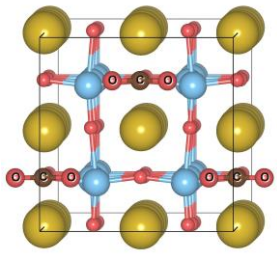
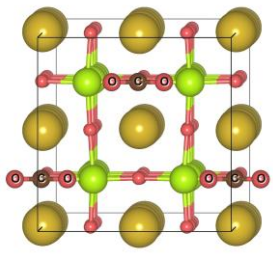
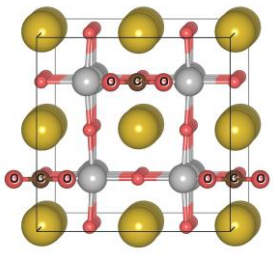
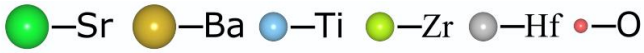
AO-terminated (001)			
BO_2-terminated (001)			
			

Figure S9. Surface relaxations of all considered perovskite surfaces upon CO_2 adsorption at Θ=0.50 coverage.

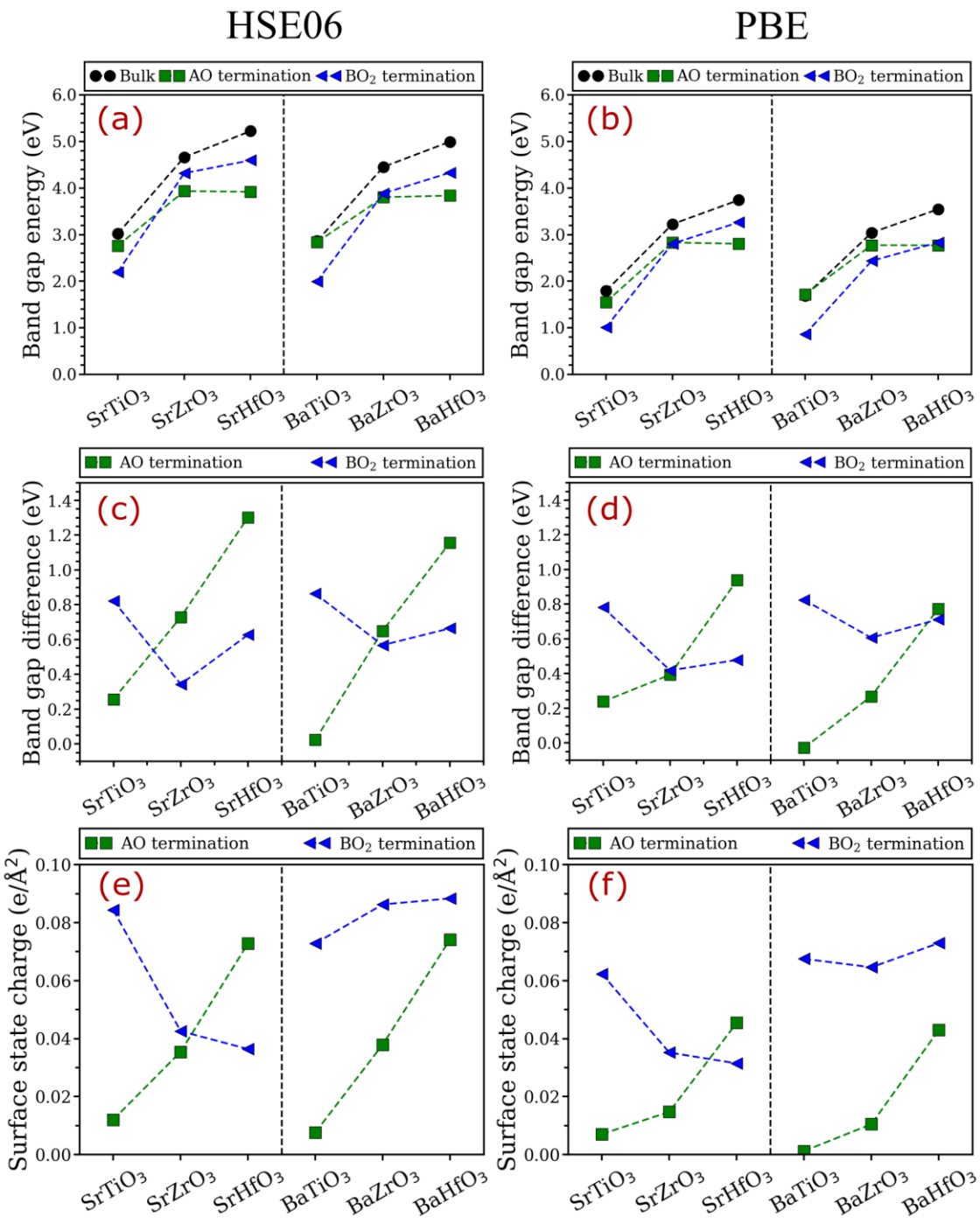


Figure S10. Comparison of (a,b) band gap energies, (c,d) band gap reductions, and (e,f) cumulative charges for the surface states at the cubic perovskites computed using (a,c,e) hybrid HSE06 and (b,d,f) PBE functionals. The HSE06 calculations were carried out using 2×2×1 Monkhorst-Pack grid on the structures optimized with PBE functional. Hafnium $5d^2 6s^2$, zirconium $4d^2 5s^2$, and titanium $3d^2 4s^2$ electrons treated explicitly for the HSE06 analysis. All other parameters were identical in both HSE06 and PBE calculations (see methods).

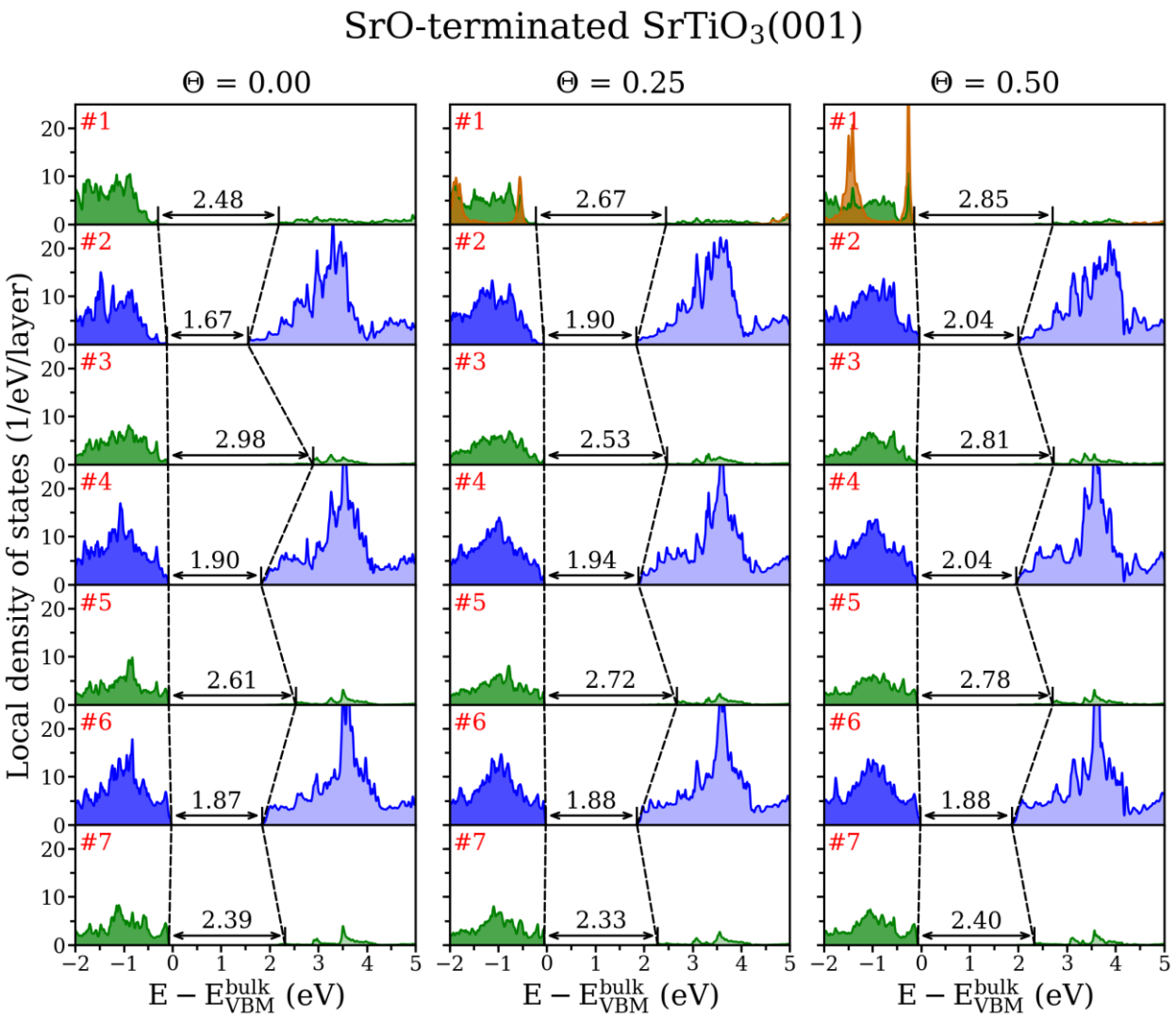


Figure S11. Layer-resolved local density of states (LDOS) for SrO-terminated $SrTiO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

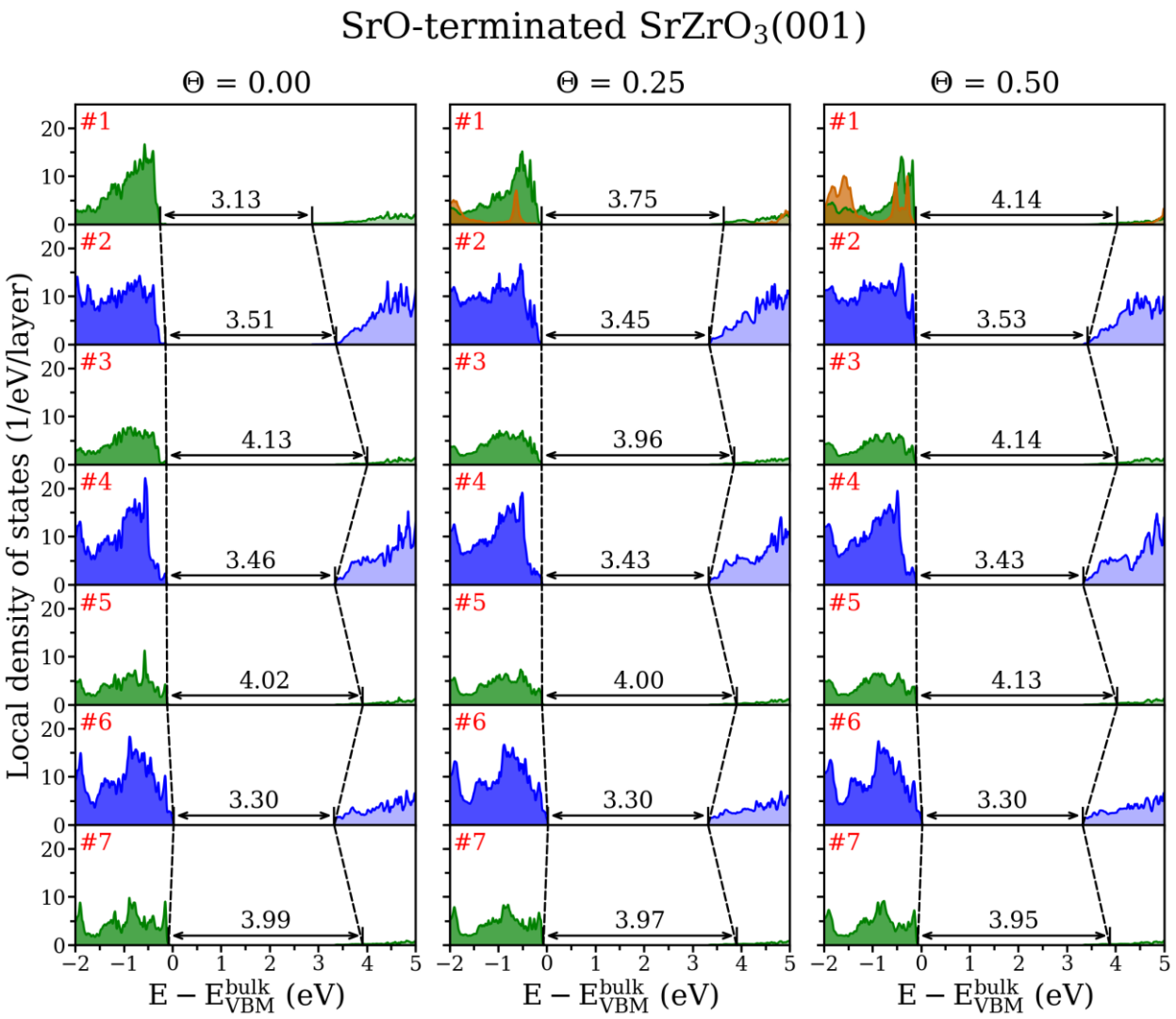


Figure S12. Layer-resolved local density of states (LDOS) for SrO-terminated $SrZrO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

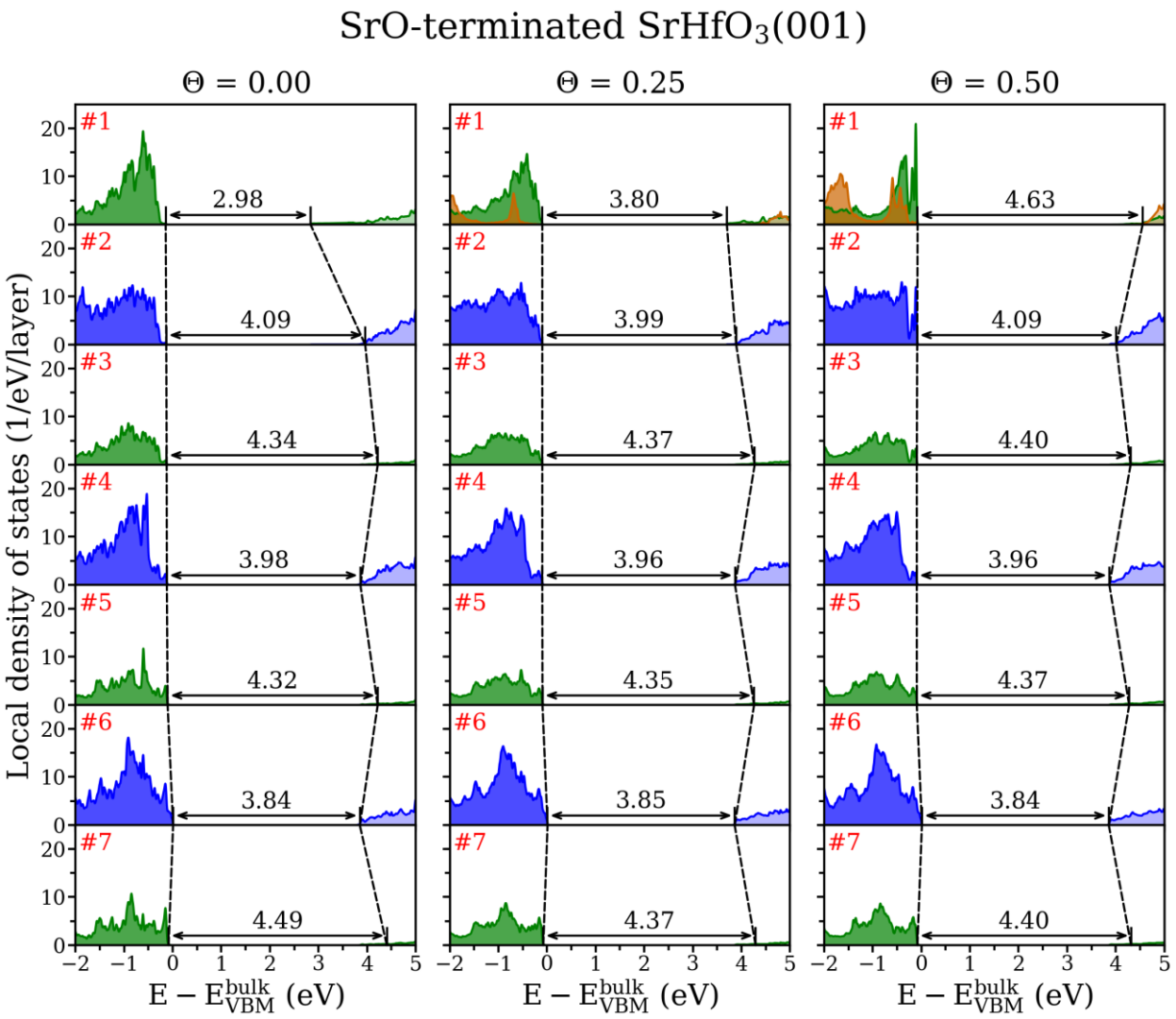


Figure S13. Layer-resolved local density of states (LDOS) for SrO-terminated $SrHfO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

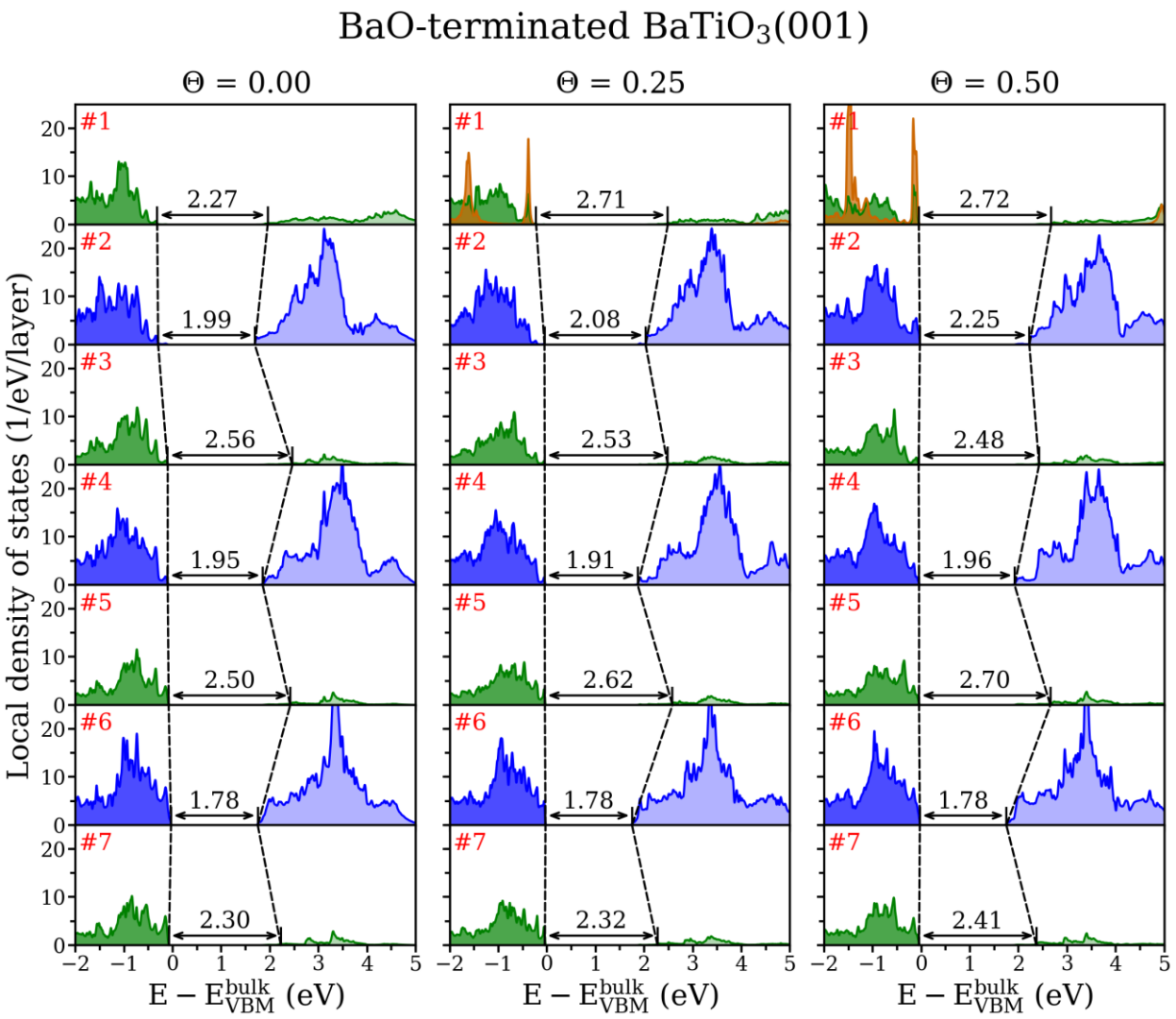


Figure S14. Layer-resolved local density of states (LDOS) for BaO-terminated $BaTiO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

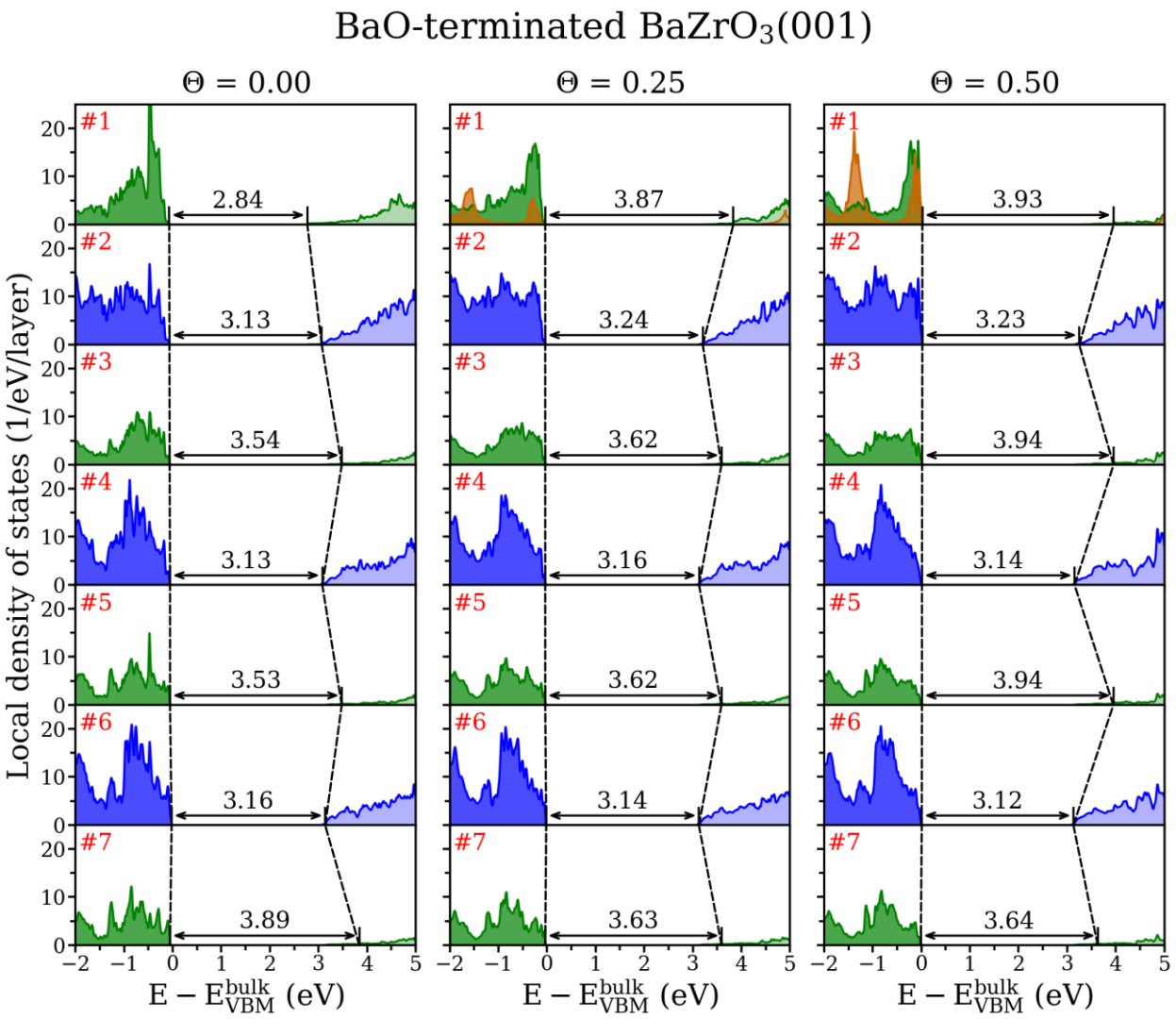


Figure S15. Layer-resolved local density of states (LDOS) for BaO-terminated $BaZrO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

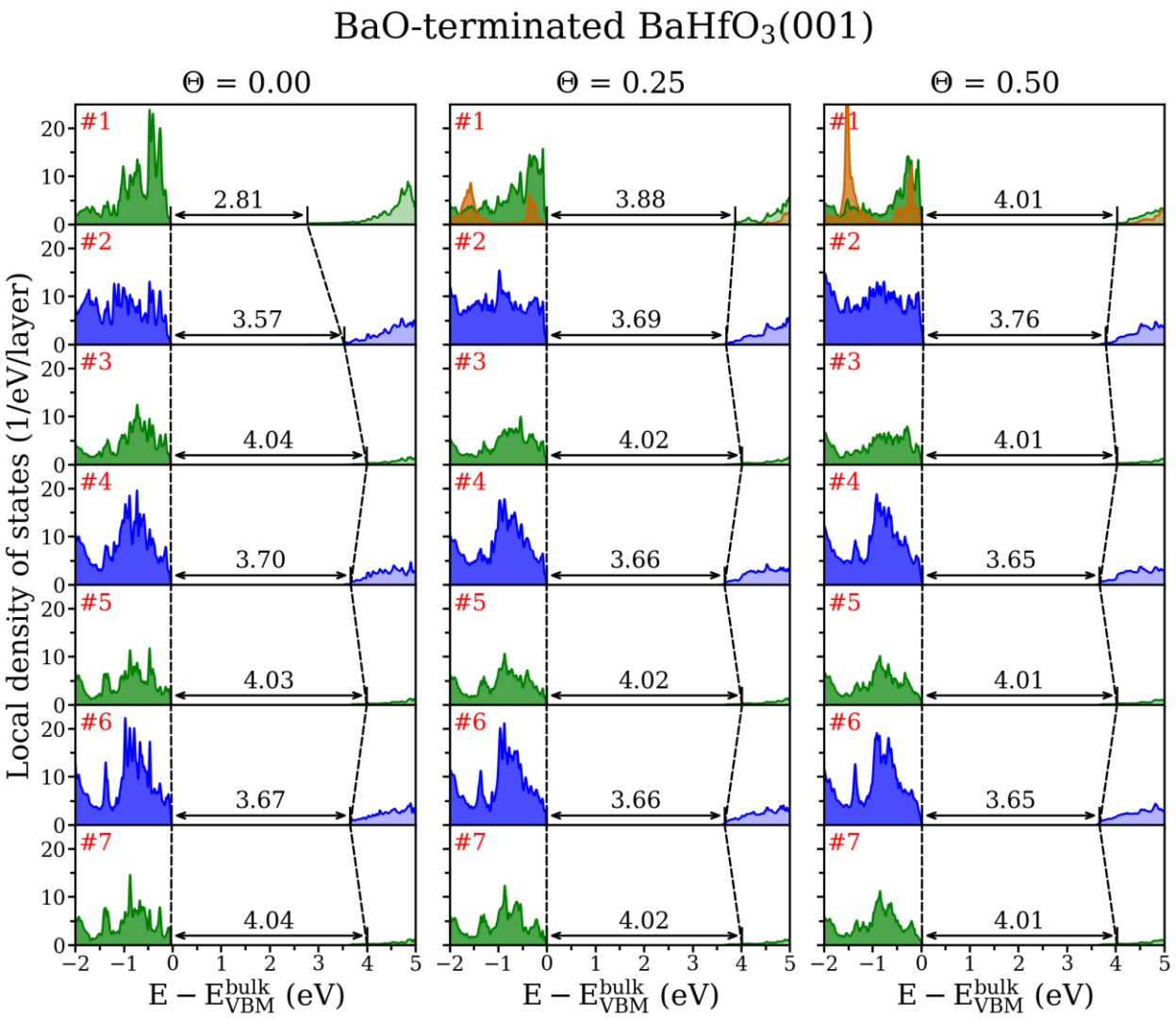


Figure S16. Layer-resolved local density of states (LDOS) for BaO-terminated $BaHfO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

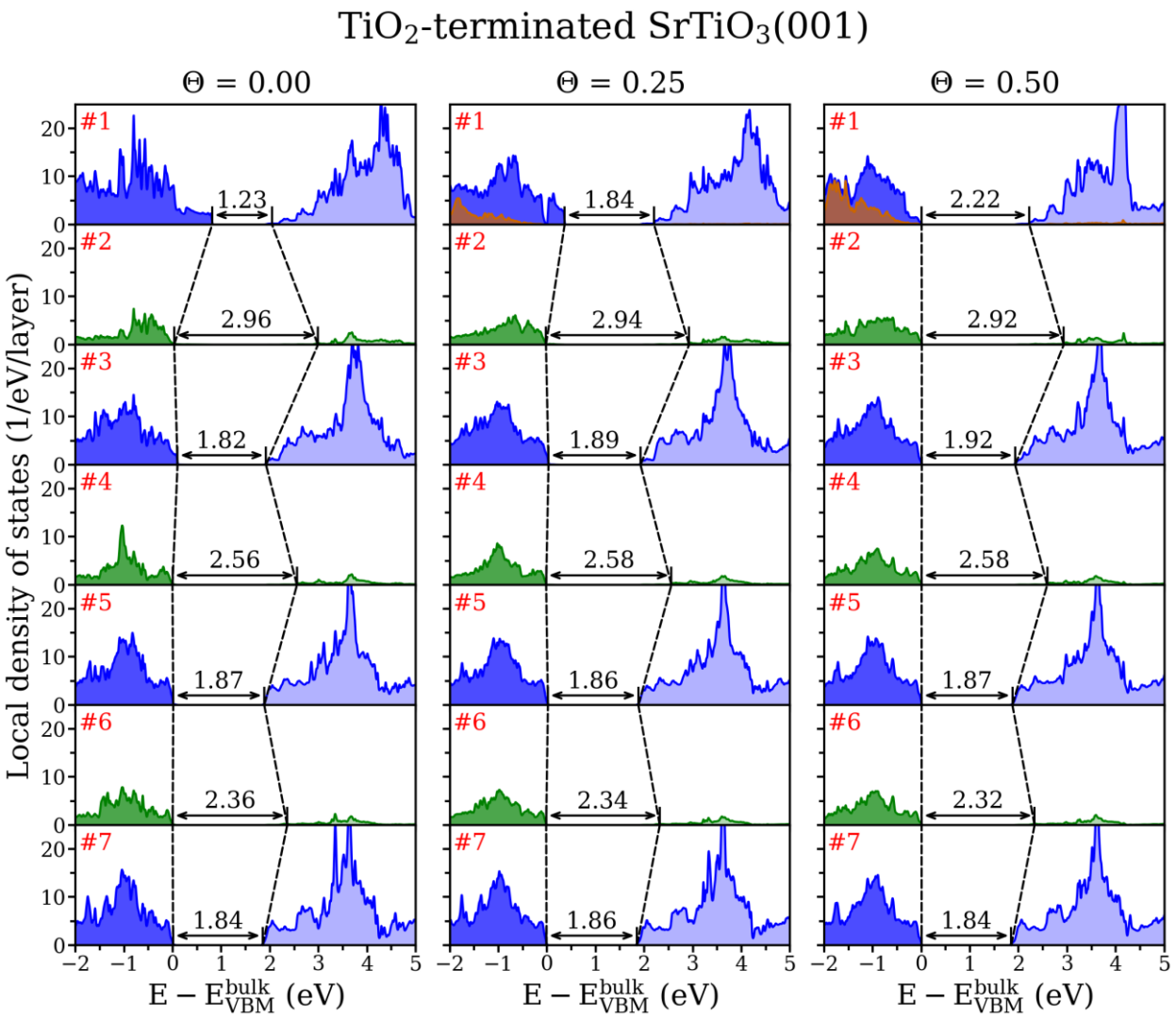


Figure S17. Layer-resolved local density of states (LDOS) for TiO_2-terminated $SrTiO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

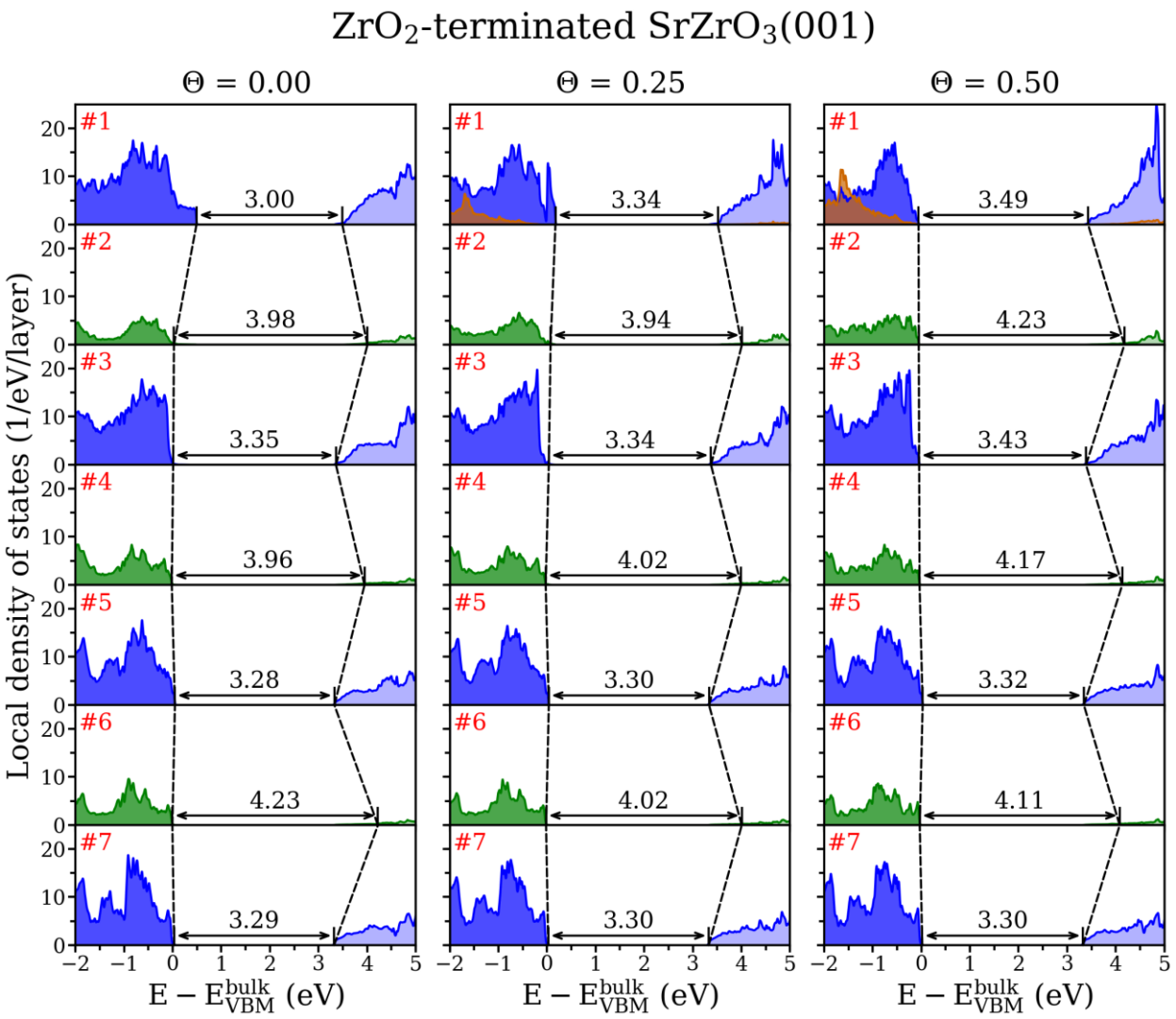


Figure S18. Layer-resolved local density of states (LDOS) for ZrO_2-terminated $SrZrO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

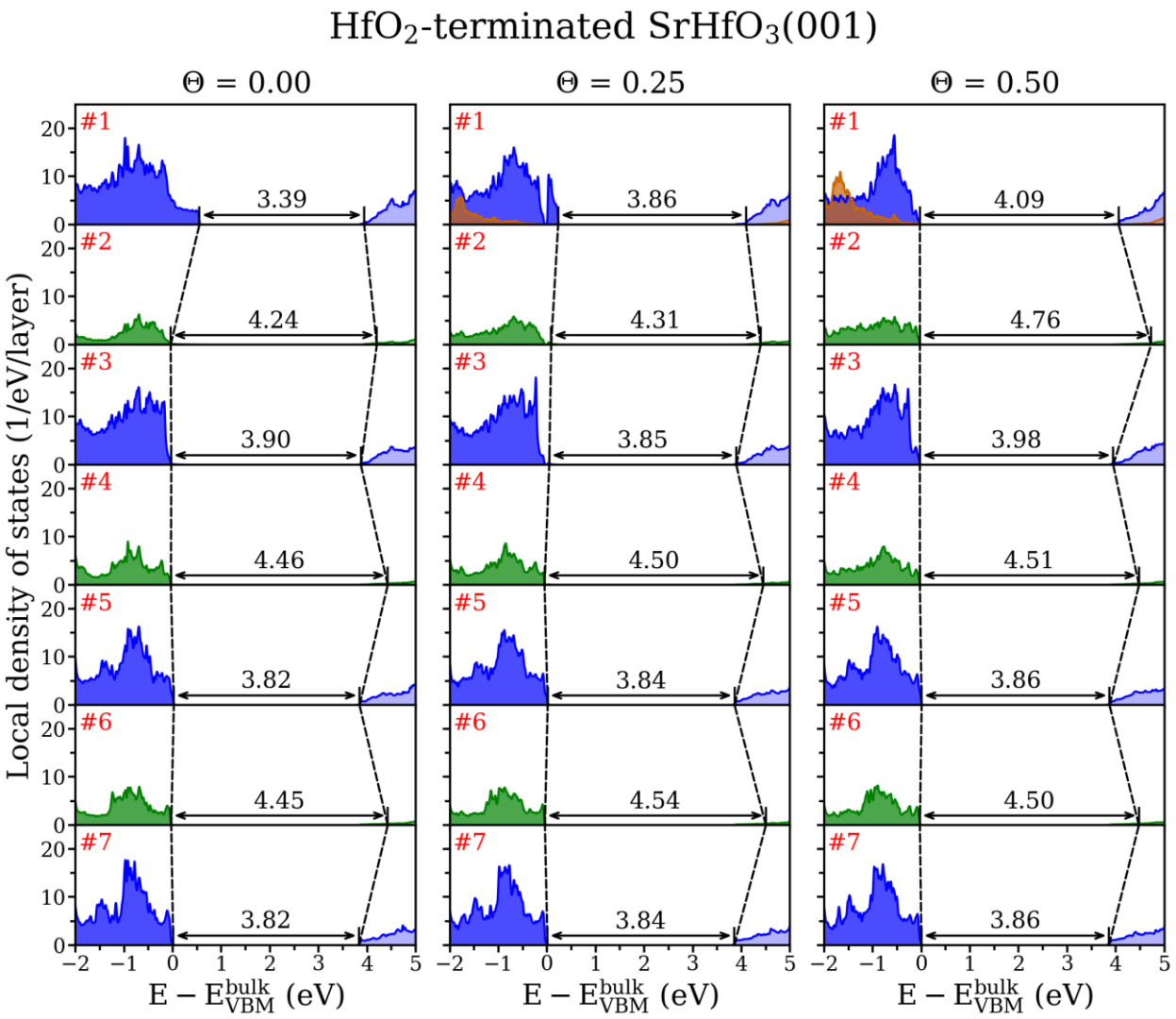


Figure S19. Layer-resolved local density of states (LDOS) for HfO_2-terminated $SrHfO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

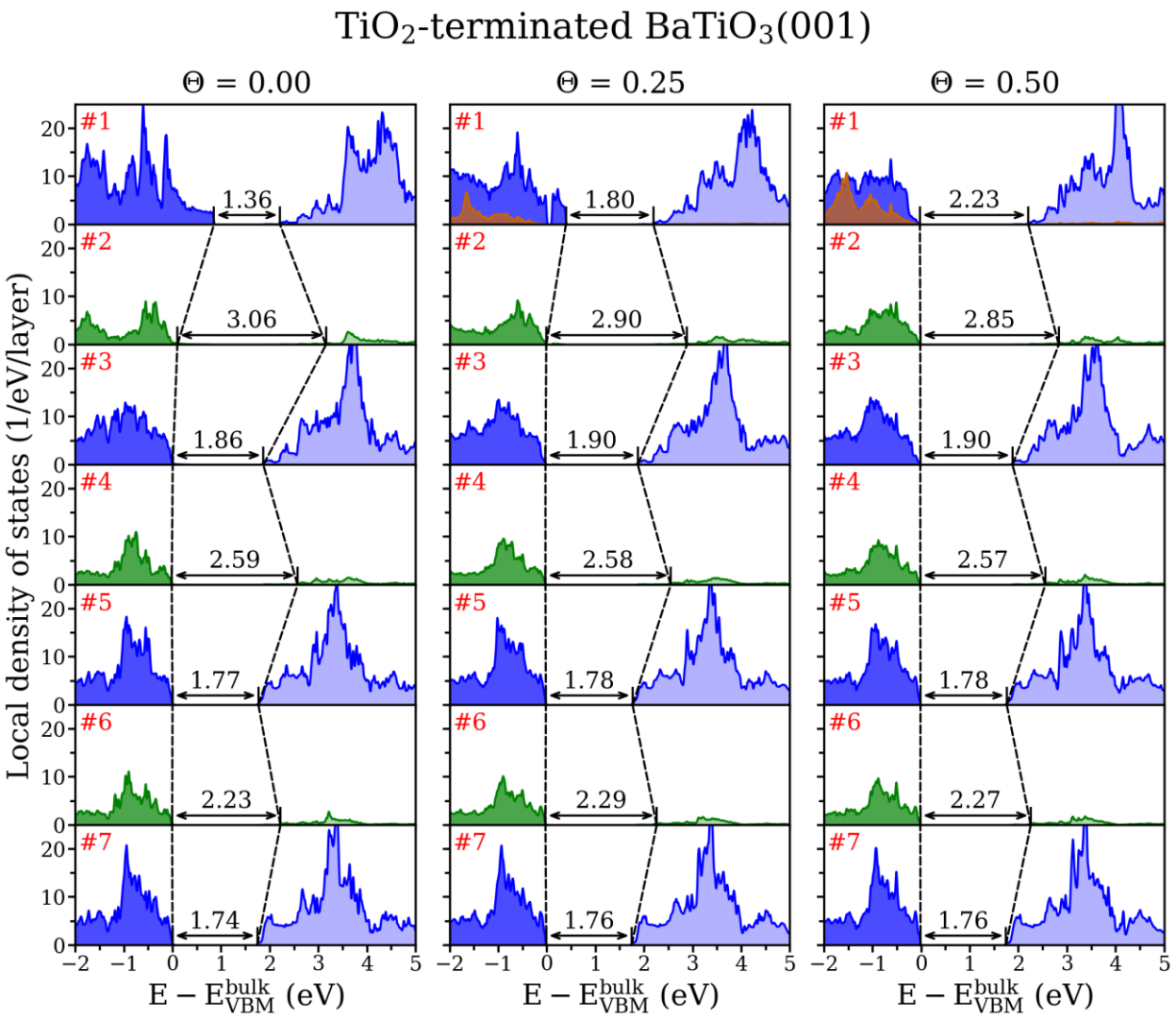


Figure S20. Layer-resolved local density of states (LDOS) for TiO_2-terminated $BaTiO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

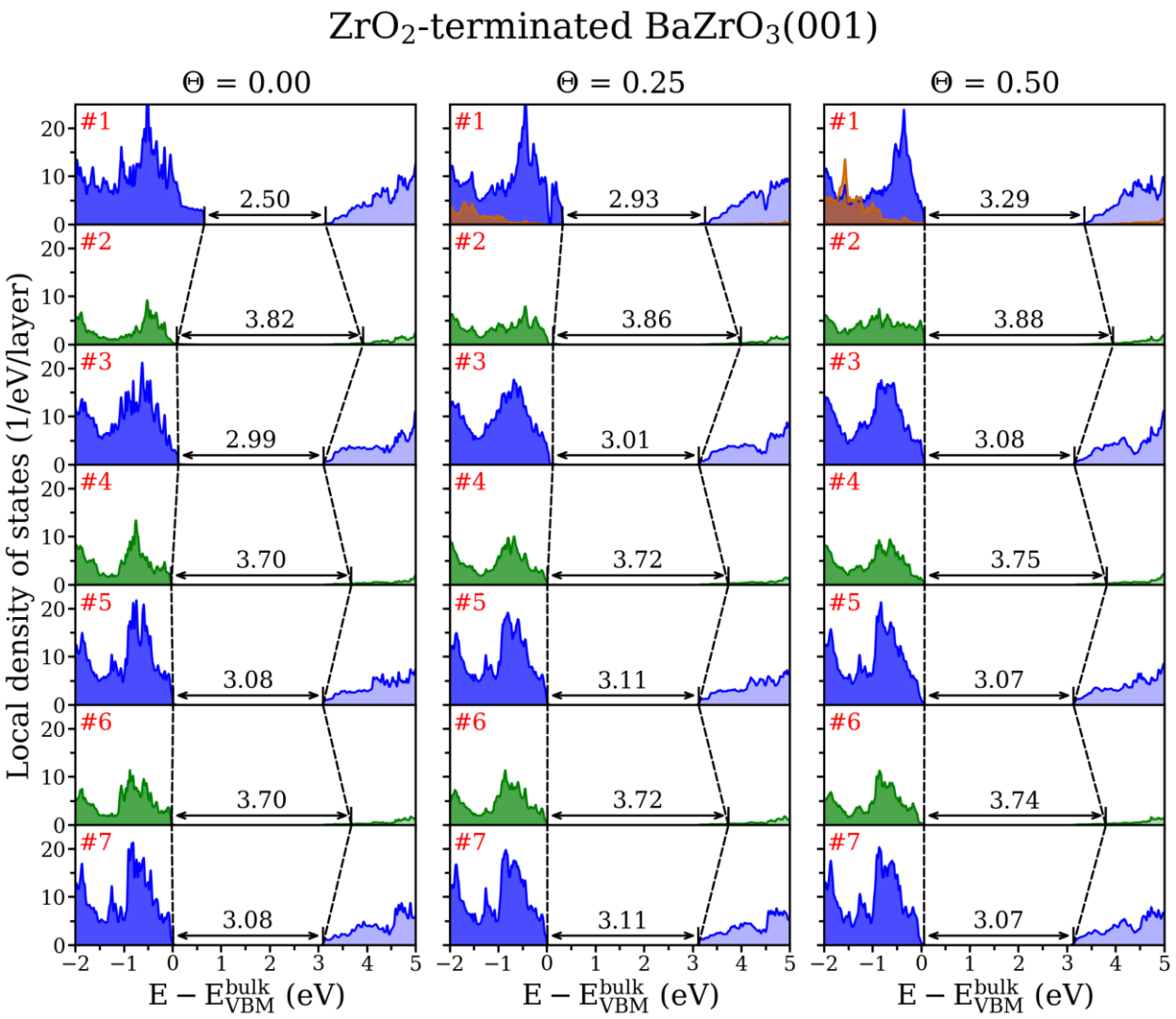


Figure S21. Layer-resolved local density of states (LDOS) for ZrO_2-terminated $BaZrO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

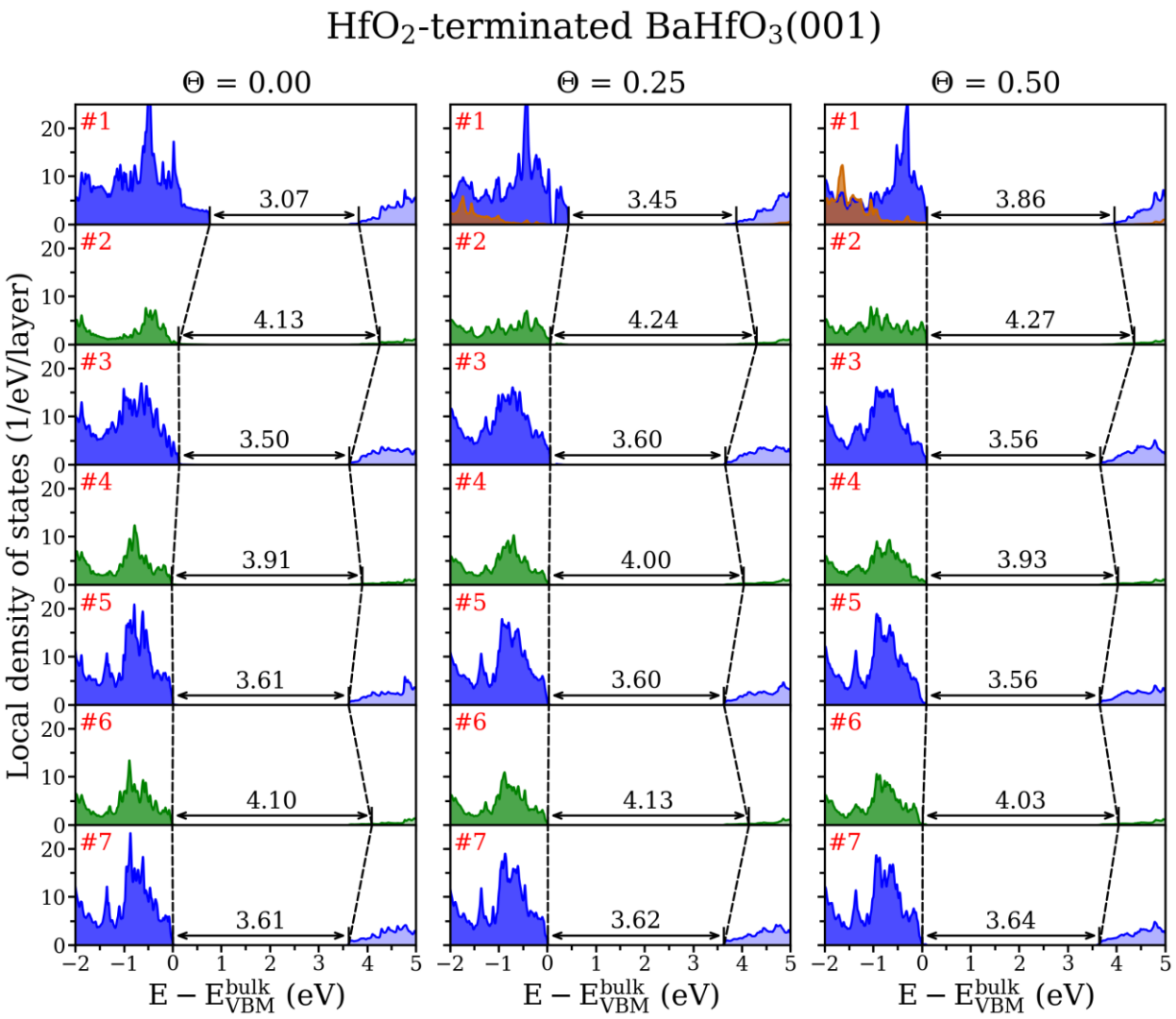


Figure S22. Layer-resolved local density of states (LDOS) for HfO_2-terminated $BaHfO_3$(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages (only one half of the slab is presented due to the symmetry; indexing is from the surface to the middle layers; numbers represent effective band gaps for the atomic layers computed form LDOS neglecting the population densities below 0.3 1/eV/layer).

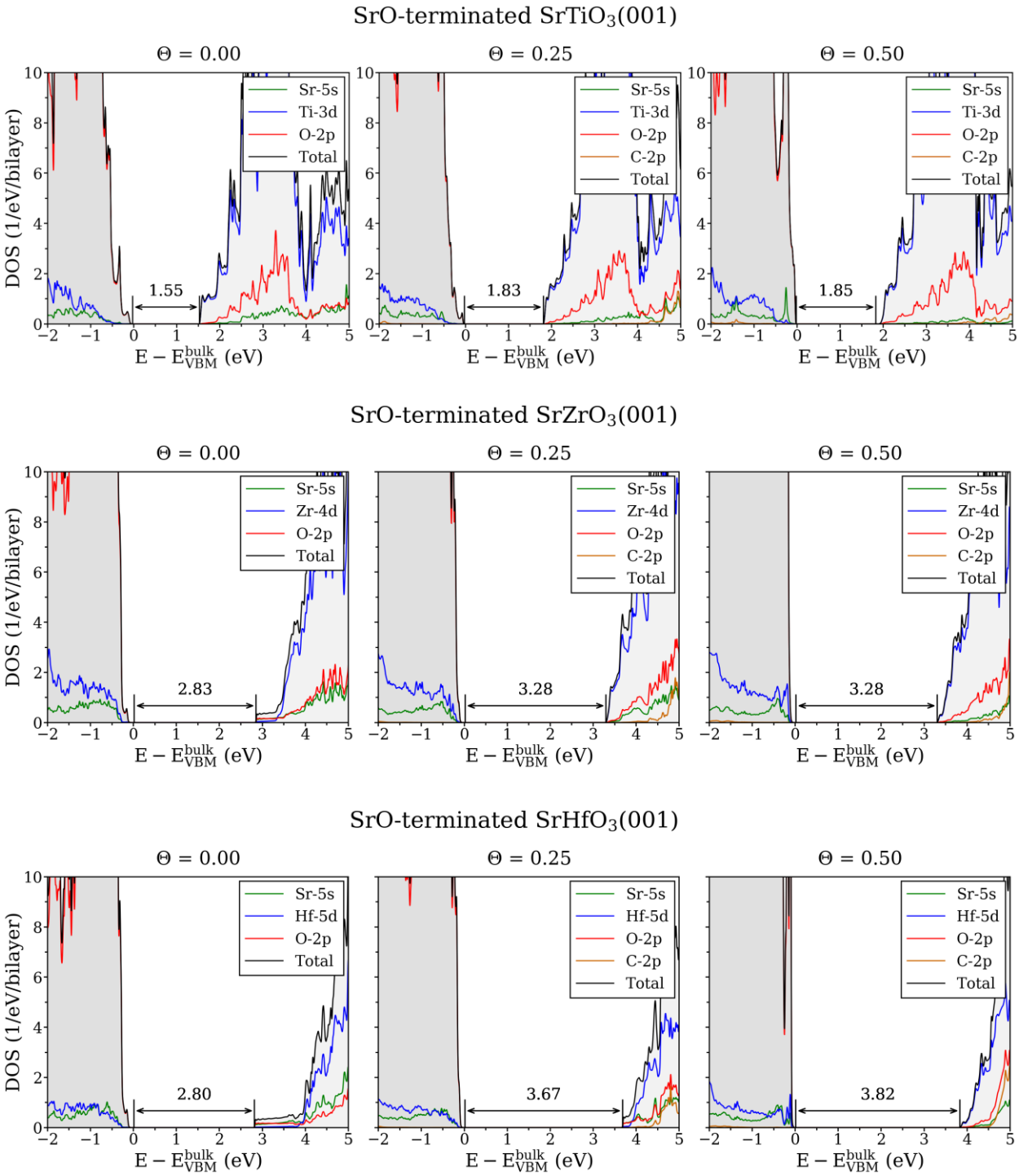


Figure S23. Projected density of states (DOS) for two surface layers of the Sr-containing AO-terminated ABO_3(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages. The numbers represent band gap energies of the slab systems.

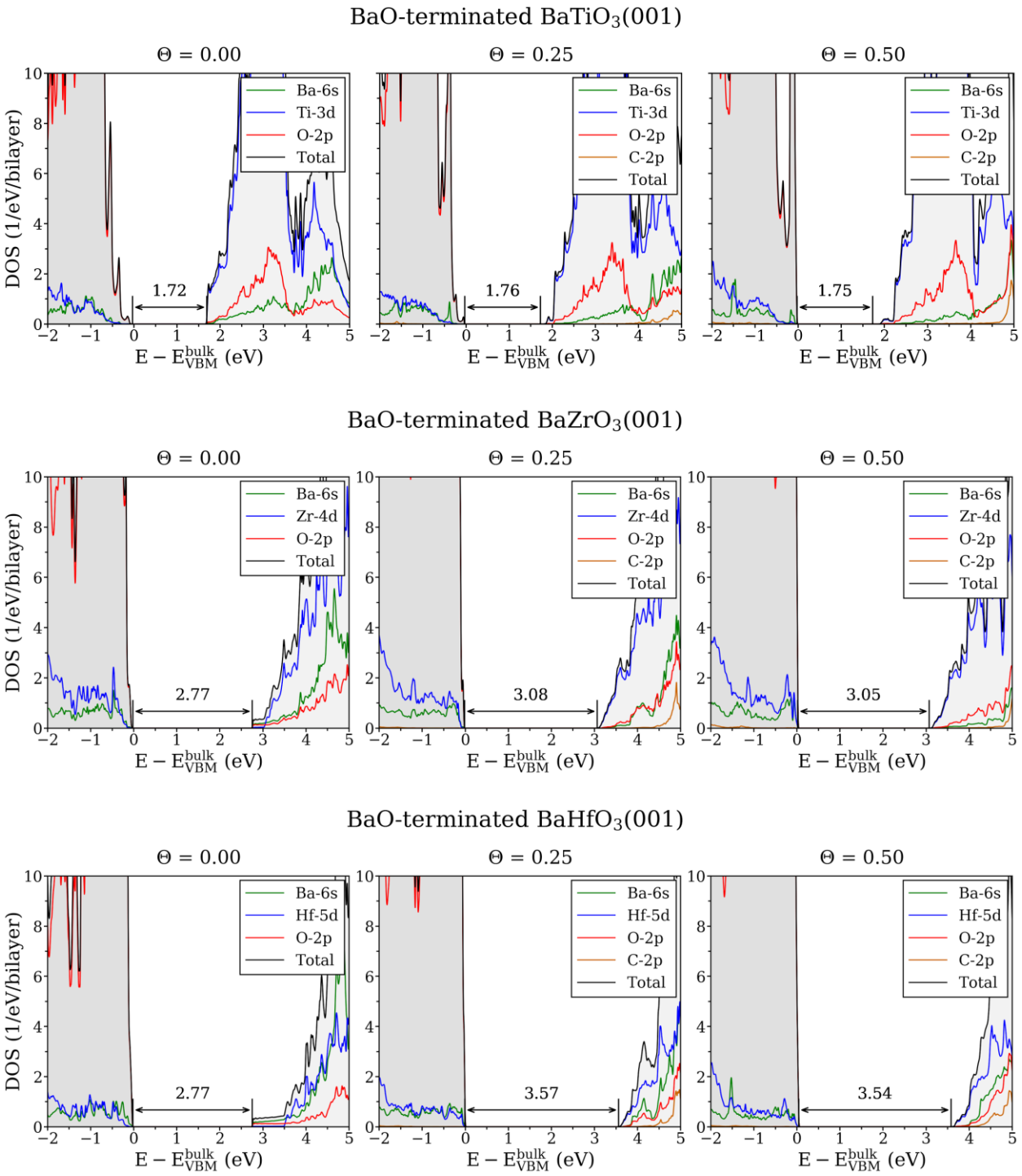


Figure S24. Projected density of states (DOS) for two surface layers of the Ba-containing AO-terminated $ABO_3(001)$ at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages. The numbers represent band gap energies of the slab systems.

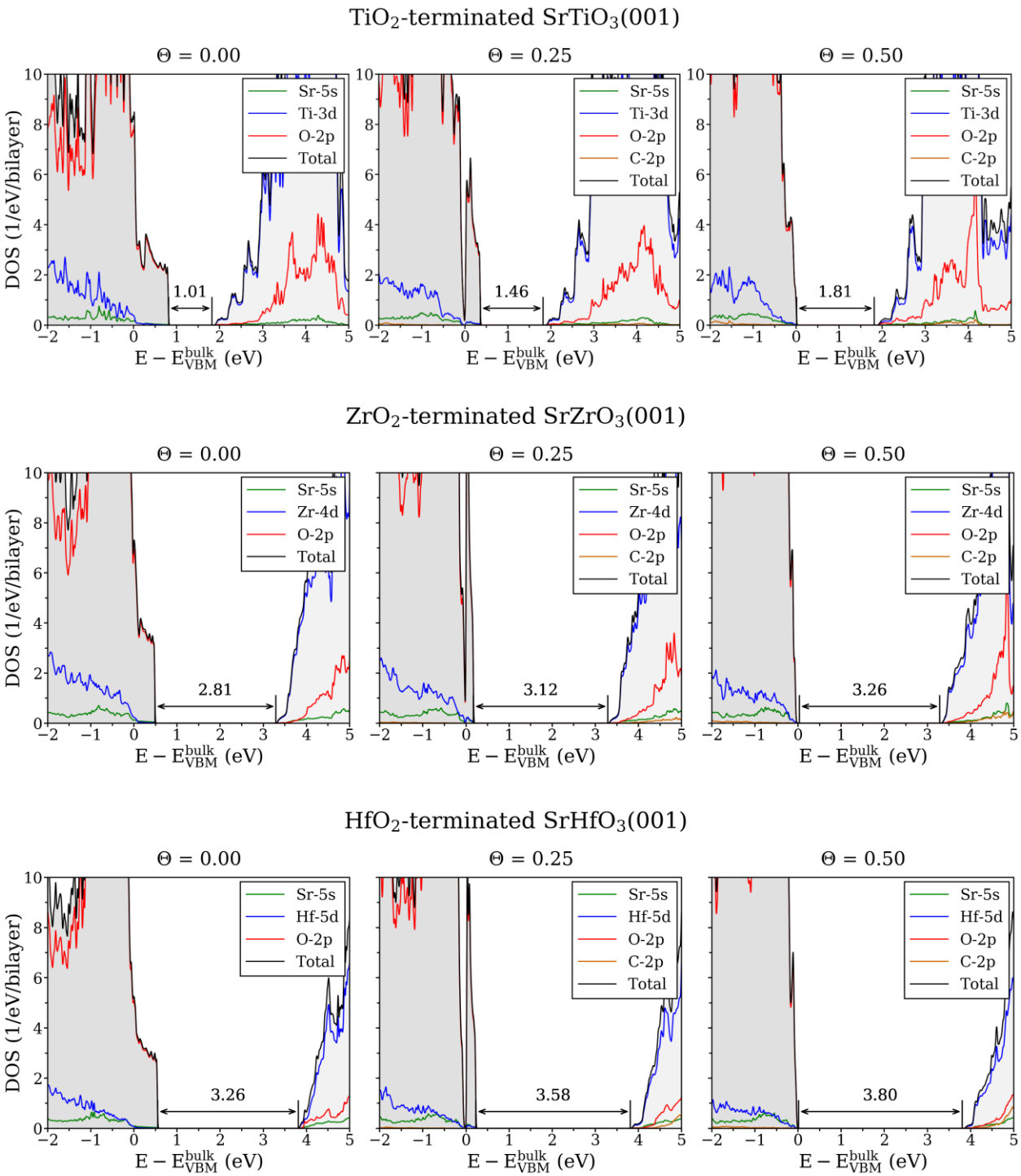


Figure S25. Projected density of states (DOS) for two surface layers of the Sr-containing BO_2-terminated ABO_3(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages. The numbers represent band gap energies of the slab systems.

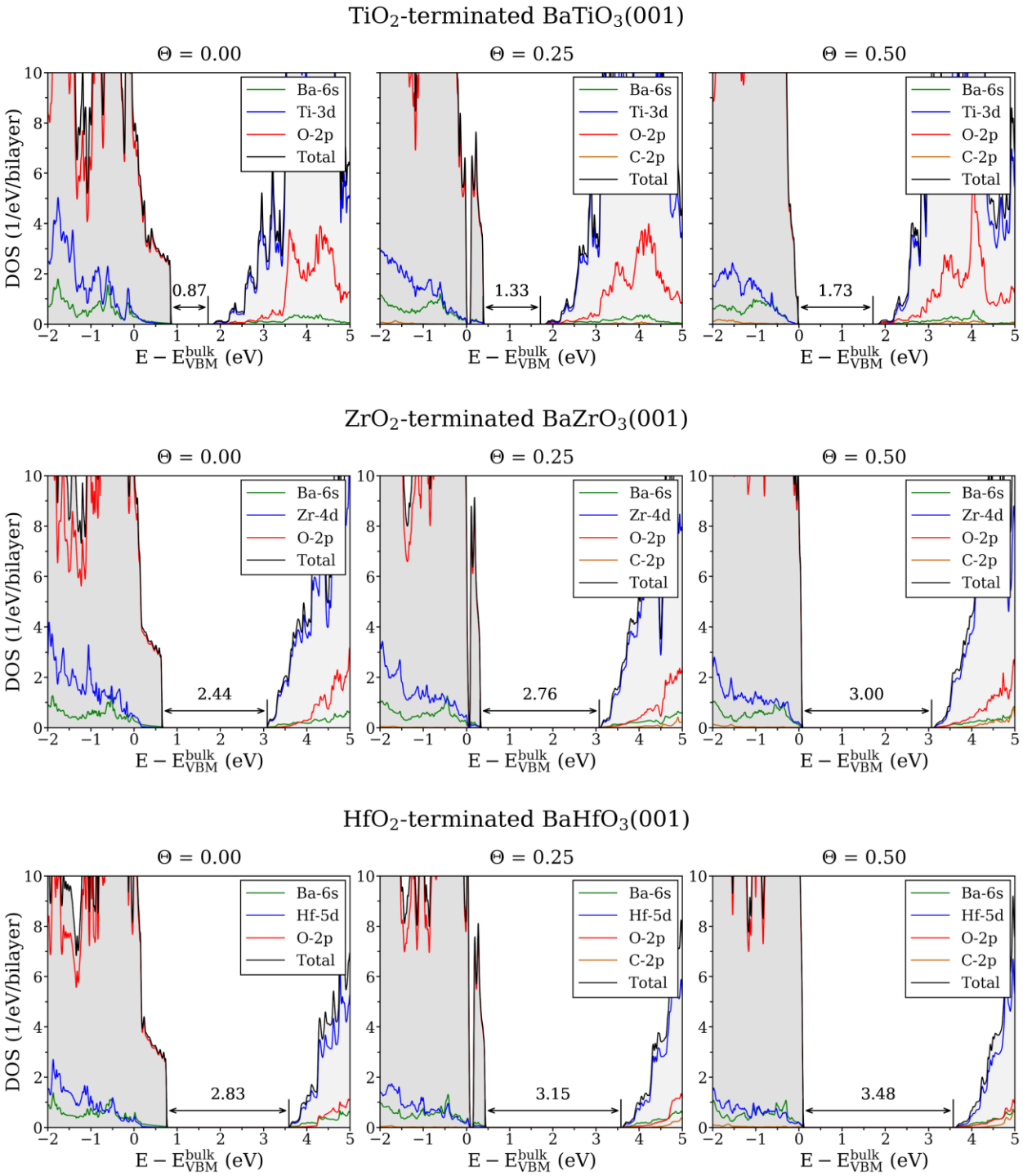


Figure S26. Projected density of states (DOS) for two surface layers of the Ba-containing BO_2-terminated ABO_3(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO_2 coverages. The numbers represent band gap energies of the slab systems.

Structure 1. SrO-terminated $SrTiO_3$ slab at Θ=0.00 CO_2 coverage

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Structure 2. SrO-terminated $SrTiO_3$ slab at Θ=0.25 CO_2 coverage

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  Sr  0.489349  0.011608  0.230341
  Sr  0.002269  0.008371  0.318484
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Ti 0.248255 0.251970 0.636456
Ti 0.244262 0.753075 0.637459
Ti 0.747169 0.255935 0.637464
Ti 0.748356 0.752031 0.723850
Ti 0.247512 0.253407 0.729554
Ti 0.246156 0.750961 0.730794
Ti 0.749972 0.254607 0.730819
C 0.793181 0.707221 0.197485
C 0.793181 0.707221 0.802515
O 0.942299 0.760424 0.190324
O 0.741145 0.557654 0.190335
O 0.698745 0.800839 0.216359
O 0.247085 0.252757 0.226540
O 0.753884 0.220707 0.227456
O 0.278820 0.745087 0.227457
O 0.753984 0.504143 0.265726
O 0.995878 0.749596 0.265839
O 0.500659 0.252356 0.271787
O 0.251089 0.999166 0.271803
O 0.000333 0.249683 0.272925
O 0.246586 0.499480 0.272958
O 0.506299 0.745280 0.274438
O 0.750642 0.993635 0.274497
O 0.769586 0.730304 0.317388
O 0.748569 0.262440 0.318152
O 0.237722 0.751355 0.318166
O 0.253192 0.246645 0.318358
O 0.752617 0.995804 0.361848
O 0.504094 0.748936 0.361860
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O 0.001430 0.248447 0.363347
O 0.501403 0.246625 0.363871
O 0.251502 0.998497 0.363879
O 0.000266 0.747465 0.364723

O 0.750590 0.499653 0.364725
O 0.250071 0.249929 0.409118
O 0.250071 0.749786 0.409118
O 0.750214 0.249929 0.409118
O 0.750214 0.749786 0.409118
O 0.250071 0.000000 0.454560
O 0.250071 0.499857 0.454560
O 0.750214 0.000000 0.454560
O 0.750214 0.499857 0.454560
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O 0.500000 0.249929 0.454560
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O 0.000143 0.249929 0.454560
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O 0.250071 0.749786 0.499998
O 0.750214 0.249929 0.499998
O 0.750214 0.749786 0.499998
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O 0.750214 0.000000 0.545440
O 0.750214 0.499857 0.545440
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O 0.500000 0.749786 0.545440
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O 0.000143 0.749786 0.545440
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O 0.250071 0.749786 0.590882
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O 0.501403 0.246625 0.636129
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O 0.752617 0.995804 0.638152
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O 0.506299 0.745280 0.725562
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O 0.000333 0.249683 0.727075
O 0.251089 0.999166 0.728197

O 0.500659 0.252356 0.728213
O 0.995878 0.749596 0.734161
O 0.753984 0.504143 0.734274
O 0.278820 0.745087 0.772543
O 0.753884 0.220707 0.772544
O 0.247085 0.252757 0.773460
O 0.698745 0.800839 0.783641
O 0.741145 0.557654 0.809666
O 0.942299 0.760424 0.809676

Structure 3. SrO-terminated $SrTiO_3$ slab at Θ=0.50 CO_2 coverage

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_cell_length_b   7.89043600
_cell_length_c   43.39739600
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.506888  0.517683  0.776161
  Sr  0.005550  0.478892  0.775658
  Sr  0.493023  0.007957  0.772575
  Sr  0.993277  0.989533  0.772324
  Sr  0.502627  0.498592  0.682868
  Sr  0.500478  0.996493  0.682463
  Sr  0.000915  0.494365  0.682291
  Sr  0.001787  0.995832  0.682158
  Sr  0.000000  0.000000  0.590881
  Sr  0.000000  0.499857  0.590881
  Sr  0.499857  0.000000  0.590881
  Sr  0.499857  0.499857  0.590881
  Sr  0.000000  0.000000  0.499998
  Sr  0.000000  0.499857  0.499998
  Sr  0.499857  0.499857  0.499998
  Sr  0.499857  0.000000  0.499998
  Sr  0.499857  0.499857  0.409119
  Sr  0.499857  0.000000  0.409119
  Sr  0.000000  0.499857  0.409119
  Sr  0.000000  0.000000  0.409119
  Sr  0.001787  0.995832  0.317842
  Sr  0.000915  0.494365  0.317709
  Sr  0.500478  0.996493  0.317537
  Sr  0.502627  0.498592  0.317132
  Sr  0.993277  0.989533  0.227676
  Sr  0.493023  0.007957  0.227425
  Sr  0.005550  0.478892  0.224342
  Sr  0.506888  0.517683  0.223839
  Ti  0.250132  0.744449  0.731882
  Ti  0.749600  0.250648  0.731745
  Ti  0.749344  0.749499  0.725011
  Ti  0.248482  0.246580  0.724914
  Ti  0.252121  0.742821  0.637989
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Ti 0.752350 0.244568 0.637976
Ti 0.256278 0.246458 0.635136
Ti 0.756156 0.744251 0.635101
Ti 0.249929 0.249929 0.545440
Ti 0.249929 0.749786 0.545440
Ti 0.749786 0.249929 0.545440
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Ti 0.749786 0.749786 0.454560
Ti 0.749786 0.249929 0.454560
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Ti 0.256278 0.246458 0.364864
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Ti 0.252121 0.742821 0.362011
Ti 0.248482 0.246580 0.275086
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Ti 0.749600 0.250648 0.268255
Ti 0.250132 0.744449 0.268118
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O 0.995806 0.743747 0.733145
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O 0.245468 0.003291 0.726005
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O 0.003577 0.256823 0.725212
O 0.503563 0.751000 0.724944
O 0.766419 0.739359 0.682717
O 0.265009 0.261359 0.682668
O 0.235104 0.742527 0.681624
O 0.736264 0.259775 0.681532
O 0.499304 0.732614 0.638123
O 0.999222 0.232137 0.638076
O 0.727387 0.000533 0.637459
O 0.268037 0.004434 0.637434
O 0.226226 0.500493 0.635924
O 0.769028 0.503868 0.635844
O 0.996519 0.774708 0.635310

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O 0.749786 0.249929 0.590881
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O 0.249929 0.499857 0.545440
O 0.749786 0.000000 0.545440
O 0.749786 0.499857 0.545440
O 0.000000 0.749786 0.545440
O 0.000000 0.249929 0.545440
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O 0.499857 0.749786 0.545440
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O 0.249929 0.249929 0.409119
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O 0.996519 0.774708 0.364690
O 0.769028 0.503868 0.364156
O 0.226226 0.500493 0.364076
O 0.268037 0.004434 0.362566
O 0.727387 0.000533 0.362541
O 0.999222 0.232137 0.361924
O 0.499304 0.732614 0.361877
O 0.736264 0.259775 0.318468
O 0.235104 0.742527 0.318376
O 0.265009 0.261359 0.317332
O 0.766419 0.739359 0.317283
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O 0.003577 0.256823 0.274788
O 0.753824 0.996356 0.274063
O 0.245468 0.003291 0.273995
O 0.744948 0.503493 0.268196

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O 0.495941 0.247593 0.267341
O 0.995806 0.743747 0.266855
O 0.776741 0.229830 0.227594
O 0.277534 0.769762 0.227545
O 0.709609 0.788564 0.220034
O 0.209282 0.209090 0.219885
O 0.248498 0.435209 0.189066
O 0.751135 0.563681 0.189032
O 0.431161 0.215962 0.186932
O 0.929143 0.786809 0.186506
O 0.929143 0.786809 0.813494
O 0.431161 0.215962 0.813068
O 0.751135 0.563681 0.810968
O 0.248498 0.435209 0.810934

Structure 4. SrO-terminated $SrZrO_3$ slab at Θ=0.00 CO_2 coverage

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_cell_length_b   8.39465800
_cell_length_c   46.17061600
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
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  Sr  0.000000  0.500000  0.500000
  Sr  0.500000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.500000  0.500000  0.590909
  Sr  0.505364  0.495239  0.680163
  Sr  0.465410  0.489142  0.766726
  Sr  0.500000  0.000000  0.590909
  Sr  0.493708  0.003240  0.680169
  Sr  0.489626  0.964777  0.766721
  Sr  0.000000  0.500000  0.590909
  Sr  0.993590  0.503513  0.680183
  Sr  0.989357  0.465093  0.766661
  Sr  0.000000  0.000000  0.590909
  Sr  0.005599  0.995257  0.680219
  Sr  0.965637  0.989622  0.766745
  Sr  0.500000  0.500000  0.409091
  Sr  0.505364  0.495239  0.319837
  Sr  0.465410  0.489142  0.233274
  Sr  0.500000  0.000000  0.409091
  Sr  0.493708  0.003240  0.319831
  Sr  0.489626  0.964777  0.233279
  Sr  0.000000  0.500000  0.409091
  Sr  0.993590  0.503513  0.319817
  Sr  0.989357  0.465093  0.233339
  Sr  0.000000  0.000000  0.409091
  Sr  0.005599  0.995257  0.319781
  Sr  0.965637  0.989622  0.233255
  Zr  0.750000  0.750000  0.545455
  Zr  0.752429  0.749369  0.636200
  Zr  0.744661  0.744933  0.727276
  Zr  0.750000  0.250000  0.545455
  Zr  0.749345  0.252285  0.636205
```

Zr 0.745320 0.243827 0.727252
Zr 0.250000 0.750000 0.545455
Zr 0.249409 0.752306 0.636197
Zr 0.245499 0.743820 0.727239
Zr 0.250000 0.250000 0.545455
Zr 0.252480 0.249339 0.636209
Zr 0.244565 0.244874 0.727273
Zr 0.750000 0.750000 0.454545
Zr 0.752429 0.749369 0.363800
Zr 0.744661 0.744933 0.272724
Zr 0.750000 0.250000 0.454545
Zr 0.749345 0.252285 0.363795
Zr 0.745320 0.243827 0.272748
Zr 0.250000 0.750000 0.454545
Zr 0.249409 0.752306 0.363803
Zr 0.245499 0.743820 0.272761
Zr 0.250000 0.250000 0.454545
Zr 0.252480 0.249339 0.363791
Zr 0.244565 0.244874 0.272727
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O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.500000 0.750000 0.545455
O 0.500728 0.700015 0.637816
O 0.501773 0.801961 0.721460
O 0.500000 0.250000 0.545455
O 0.500338 0.307767 0.634070
O 0.500090 0.199881 0.731772
O 0.000000 0.750000 0.545455
O 0.000368 0.807686 0.634130
O 0.000198 0.699620 0.731544
O 0.000000 0.250000 0.545455
O 0.000715 0.200069 0.637897
O 0.001672 0.301793 0.721373
O 0.750000 0.750000 0.590909
O 0.774332 0.723556 0.681350
O 0.733638 0.802240 0.770683
O 0.750000 0.250000 0.590909
O 0.726136 0.277089 0.681377
O 0.802410 0.232305 0.770664
O 0.250000 0.750000 0.590909
O 0.227111 0.777511 0.681366
O 0.302182 0.732166 0.770663
O 0.250000 0.250000 0.590909
O 0.275022 0.223442 0.681359

O 0.232933 0.302252 0.770668
O 0.750000 0.500000 0.545455
O 0.807622 0.500332 0.633891
O 0.701082 0.499503 0.732011
O 0.750000 0.000000 0.545455
O 0.699898 0.000749 0.637977
O 0.802974 0.001018 0.721287
O 0.250000 0.500000 0.545455
O 0.199969 0.500769 0.638032
O 0.303015 0.500975 0.721270
O 0.250000 0.000000 0.545455
O 0.307587 0.000380 0.633857
O 0.200919 0.999478 0.731983
O 0.500000 0.750000 0.454545
O 0.500728 0.700015 0.362184
O 0.501773 0.801961 0.278540
O 0.500000 0.250000 0.454545
O 0.500338 0.307767 0.365930
O 0.500090 0.199881 0.268228
O 0.000000 0.750000 0.454545
O 0.000368 0.807686 0.365870
O 0.000198 0.699620 0.268456
O 0.000000 0.250000 0.454545
O 0.000715 0.200069 0.362103
O 0.001672 0.301793 0.278627
O 0.750000 0.750000 0.409091
O 0.774332 0.723556 0.318650
O 0.733638 0.802240 0.229317
O 0.750000 0.250000 0.409091
O 0.726136 0.277089 0.318623
O 0.802410 0.232305 0.229336
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O 0.227111 0.777511 0.318634
O 0.302182 0.732166 0.229337
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O 0.275022 0.223442 0.318641
O 0.232933 0.302252 0.229332
O 0.750000 0.500000 0.454545
O 0.807622 0.500332 0.366109
O 0.701082 0.499503 0.267989
O 0.750000 0.000000 0.454545
O 0.699898 0.000749 0.362023
O 0.802974 0.001018 0.278713
O 0.250000 0.500000 0.454545
O 0.199969 0.500769 0.361968
O 0.303015 0.500975 0.278730

O 0.250000 0.000000 0.454545
O 0.307587 0.000380 0.366143
O 0.200919 0.999478 0.268017

Structure 5. SrO-terminated $SrZrO_3$ slab at Θ=0.25 CO_2 coverage

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_cell_length_c   46.17061600
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
_atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.009646  0.496240  0.682449
  Sr  0.063690  0.510220  0.774130
  Sr  0.512162  0.494854  0.681737
  Sr  0.516630  0.488118  0.773239
  Sr  0.999200  0.002524  0.678629
  Sr  0.970324  0.015458  0.766356
  Sr  0.481917  0.004313  0.679541
  Sr  0.491216  0.015510  0.765120
  Sr  0.500000  0.000000  0.500000
  Sr  0.000000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.000000  0.500000  0.500000
  Sr  0.000000  0.500000  0.590909
  Sr  0.500000  0.500000  0.590909
  Sr  0.000000  0.000000  0.590909
  Sr  0.500000  0.000000  0.590909
  Sr  0.009646  0.496240  0.317551
  Sr  0.063690  0.510220  0.225870
  Sr  0.512162  0.494854  0.318263
  Sr  0.516630  0.488118  0.226761
  Sr  0.999200  0.002524  0.321371
  Sr  0.970324  0.015458  0.233644
  Sr  0.481917  0.004313  0.320459
  Sr  0.491216  0.015510  0.234880
  Sr  0.000000  0.500000  0.409091
  Sr  0.500000  0.500000  0.409091
  Sr  0.000000  0.000000  0.409091
  Sr  0.500000  0.000000  0.409091
  Zr  0.251103  0.256048  0.727479
  Zr  0.749584  0.257189  0.727529
  Zr  0.255317  0.750570  0.728193
  Zr  0.752177  0.751062  0.724260
  Zr  0.250000  0.250000  0.545455
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Zr 0.750000 0.250000 0.545455
Zr 0.753238 0.252106 0.636404
Zr 0.250000 0.750000 0.545455
Zr 0.248659 0.752075 0.636607
Zr 0.750000 0.750000 0.545455
Zr 0.752702 0.747353 0.635671
Zr 0.251103 0.256048 0.272521
Zr 0.749584 0.257189 0.272471
Zr 0.255317 0.750570 0.271807
Zr 0.752177 0.751062 0.275740
Zr 0.250000 0.250000 0.454545
Zr 0.247782 0.247756 0.363774
Zr 0.750000 0.250000 0.454545
Zr 0.753238 0.252106 0.363596
Zr 0.250000 0.750000 0.454545
Zr 0.248659 0.752075 0.363393
Zr 0.750000 0.750000 0.454545
Zr 0.752702 0.747353 0.364329
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C 0.808719 0.719018 0.207148
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O 0.694103 0.505054 0.729886
O 0.219101 0.001328 0.735689
O 0.800655 0.998446 0.721737
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O 0.779000 0.281346 0.681267
O 0.714687 0.202857 0.769695
O 0.226594 0.787390 0.681484
O 0.298800 0.688785 0.769714
O 0.779779 0.716081 0.681549
O 0.000314 0.294061 0.733460
O 0.499408 0.209603 0.720153
O 0.997309 0.713506 0.734450
O 0.505235 0.804482 0.721925
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O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.250000 0.250000 0.500000
O 0.250000 0.500000 0.545455
O 0.200338 0.499662 0.638192
O 0.750000 0.500000 0.545455

O 0.802619 0.500316 0.632928
O 0.250000 0.000000 0.545455
O 0.307631 0.999805 0.633231
O 0.750000 0.000000 0.545455
O 0.702280 0.998840 0.639239
O 0.250000 0.250000 0.590909
O 0.750000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.750000 0.750000 0.590909
O 0.000000 0.250000 0.545455
O 0.999806 0.193997 0.633527
O 0.500000 0.250000 0.545455
O 0.500011 0.298187 0.638515
O 0.000000 0.750000 0.545455
O 0.999599 0.804935 0.633990
O 0.500000 0.750000 0.545455
O 0.501137 0.699229 0.638386
O 0.274401 0.501145 0.283498
O 0.694103 0.505054 0.270114
O 0.219101 0.001328 0.264311
O 0.800655 0.998446 0.278263
O 0.221425 0.213268 0.318798
O 0.779000 0.281346 0.318733
O 0.714687 0.202857 0.230305
O 0.226594 0.787390 0.318516
O 0.298800 0.688785 0.230286
O 0.779779 0.716081 0.318451
O 0.000314 0.294061 0.266540
O 0.499408 0.209603 0.279847
O 0.997309 0.713506 0.265550
O 0.505235 0.804482 0.278075
O 0.290582 0.293512 0.229100
O 0.710706 0.798128 0.225216
O 0.776388 0.573088 0.200962
O 0.937418 0.786937 0.198676
O 0.250000 0.500000 0.454545
O 0.200338 0.499662 0.361808
O 0.750000 0.500000 0.454545
O 0.802619 0.500316 0.367072
O 0.250000 0.000000 0.454545
O 0.307631 0.999805 0.366769
O 0.750000 0.000000 0.454545
O 0.702280 0.998840 0.360761
O 0.250000 0.250000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.750000 0.409091

O 0.750000 0.750000 0.409091
O 0.000000 0.250000 0.454545
O 0.999806 0.193997 0.366473
O 0.500000 0.250000 0.454545
O 0.500011 0.298187 0.361485
O 0.000000 0.750000 0.454545
O 0.999599 0.804935 0.366010
O 0.500000 0.750000 0.454545
O 0.501137 0.699229 0.361614

Structure 6. SrO-terminated $SrZrO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.39465800
_cell_length_b   8.39465800
_cell_length_c   46.17061600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.488259  0.552294  0.223789
  Sr  0.504799  0.026993  0.226473
  Sr  0.969224  0.464750  0.228811
  Sr  0.992058  0.994157  0.232747
  Sr  0.496803  0.505929  0.316756
  Sr  0.501055  0.014954  0.317392
  Sr  0.000573  0.985463  0.320300
  Sr  0.002099  0.493132  0.321582
  Sr  0.500000  0.000000  0.409091
  Sr  0.000000  0.500000  0.409091
  Sr  0.500000  0.500000  0.409091
  Sr  0.000000  0.000000  0.409091
  Sr  0.000000  0.000000  0.500000
  Sr  0.000000  0.500000  0.500000
  Sr  0.500000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.500000  0.000000  0.590909
  Sr  0.500000  0.500000  0.590909
  Sr  0.000000  0.000000  0.590909
  Sr  0.000000  0.500000  0.590909
  Sr  0.002099  0.493132  0.678418
  Sr  0.000573  0.985463  0.679700
  Sr  0.501055  0.014954  0.682608
  Sr  0.496803  0.505929  0.683244
  Sr  0.992058  0.994157  0.767253
  Sr  0.969224  0.464750  0.771189
  Sr  0.504799  0.026993  0.773527
  Sr  0.488259  0.552294  0.776210
  Zr  0.249419  0.752535  0.270993
  Zr  0.743973  0.250541  0.272363
  Zr  0.245534  0.253564  0.275415
  Zr  0.749118  0.748563  0.275817
  Zr  0.248547  0.748457  0.363175
```

Zr 0.747256 0.252858 0.363432
Zr 0.752660 0.747450 0.364246
Zr 0.253144 0.252053 0.364429
Zr 0.750000 0.750000 0.454545
Zr 0.750000 0.250000 0.454545
Zr 0.250000 0.750000 0.454545
Zr 0.250000 0.250000 0.454545
Zr 0.750000 0.750000 0.545455
Zr 0.750000 0.250000 0.545455
Zr 0.250000 0.750000 0.545455
Zr 0.250000 0.250000 0.545455
Zr 0.253144 0.252053 0.635571
Zr 0.752660 0.747450 0.635754
Zr 0.747256 0.252858 0.636568
Zr 0.248547 0.748457 0.636825
Zr 0.749118 0.748563 0.724183
Zr 0.245534 0.253564 0.724585
Zr 0.743973 0.250541 0.727637
Zr 0.249419 0.752535 0.729007
C 0.789373 0.735991 0.204379
C 0.281323 0.305875 0.206683
C 0.281323 0.305875 0.793317
C 0.789373 0.735991 0.795621
O 0.902687 0.814131 0.193441
O 0.751835 0.591832 0.197661
O 0.215509 0.436338 0.199088
O 0.424792 0.270518 0.199571
O 0.204210 0.208603 0.225313
O 0.702888 0.803044 0.226370
O 0.791914 0.209875 0.230664
O 0.319991 0.797525 0.230737
O 0.995202 0.720926 0.262651
O 0.707429 0.503405 0.266476
O 0.290670 0.497802 0.267250
O 0.494194 0.199306 0.270193
O 0.000037 0.298510 0.278129
O 0.201635 0.004252 0.278424
O 0.785766 0.996618 0.280362
O 0.503903 0.774991 0.283524
O 0.213202 0.726423 0.318496
O 0.279367 0.278002 0.318569
O 0.794412 0.717073 0.318664
O 0.717830 0.279669 0.318886
O 0.000972 0.202962 0.360753
O 0.701816 0.998867 0.361292
O 0.501655 0.699747 0.361550

O 0.300673 0.000958 0.361745
O 0.196107 0.499509 0.366107
O 0.806721 0.500101 0.366608
O 0.000123 0.808154 0.366727
O 0.499361 0.302442 0.367105
O 0.750000 0.750000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.250000 0.409091
O 0.250000 0.750000 0.409091
O 0.500000 0.750000 0.454545
O 0.500000 0.250000 0.454545
O 0.750000 0.500000 0.454545
O 0.750000 0.000000 0.454545
O 0.250000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.000000 0.250000 0.454545
O 0.000000 0.750000 0.454545
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.500000 0.750000 0.545455
O 0.500000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.000000 0.250000 0.545455
O 0.750000 0.500000 0.545455
O 0.750000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.250000 0.000000 0.545455
O 0.750000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.250000 0.250000 0.590909
O 0.499361 0.302442 0.632895
O 0.000123 0.808154 0.633273
O 0.806721 0.500101 0.633392
O 0.196107 0.499509 0.633893
O 0.300673 0.000958 0.638255
O 0.501655 0.699747 0.638450
O 0.701816 0.998867 0.638708
O 0.000972 0.202962 0.639247
O 0.717830 0.279669 0.681114
O 0.794412 0.717073 0.681336
O 0.279367 0.278002 0.681431
O 0.213202 0.726423 0.681504
O 0.503903 0.774991 0.716476

O 0.785766 0.996618 0.719638
O 0.201635 0.004252 0.721576
O 0.000037 0.298510 0.721871
O 0.494194 0.199306 0.729807
O 0.290670 0.497802 0.732750
O 0.707429 0.503405 0.733524
O 0.995202 0.720926 0.737349
O 0.319991 0.797525 0.769263
O 0.791914 0.209875 0.769336
O 0.702888 0.803044 0.773630
O 0.204210 0.208603 0.774687
O 0.424792 0.270518 0.800429
O 0.215509 0.436338 0.800912
O 0.751835 0.591832 0.802339
O 0.902687 0.814131 0.806559

Structure 7. SrO-terminated $SrHfO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.000000  0.000000  0.500000
  Sr  0.000000  0.500000  0.500000
  Sr  0.500000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.500000  0.500000  0.590909
  Sr  0.504750  0.497550  0.680668
  Sr  0.469417  0.491731  0.767919
  Sr  0.500000  0.000000  0.590909
  Sr  0.497121  0.003618  0.680698
  Sr  0.492496  0.968909  0.767943
  Sr  0.000000  0.500000  0.590909
  Sr  0.996949  0.503899  0.680690
  Sr  0.992365  0.469238  0.767883
  Sr  0.000000  0.000000  0.590909
  Sr  0.004990  0.997502  0.680716
  Sr  0.969626  0.992375  0.767940
  Sr  0.500000  0.500000  0.409091
  Sr  0.504750  0.497550  0.319332
  Sr  0.469417  0.491731  0.232082
  Sr  0.500000  0.000000  0.409091
  Sr  0.497121  0.003618  0.319302
  Sr  0.492496  0.968909  0.232057
  Sr  0.000000  0.500000  0.409091
  Sr  0.996949  0.503899  0.319310
  Sr  0.992365  0.469238  0.232117
  Sr  0.000000  0.000000  0.409091
  Sr  0.004990  0.997502  0.319284
  Sr  0.969626  0.992375  0.232060
  Hf  0.750000  0.750000  0.545455
  Hf  0.752155  0.749302  0.636299
  Hf  0.746753  0.746352  0.727657
  Hf  0.750000  0.250000  0.545455
  Hf  0.749390  0.252031  0.636306
```

Hf 0.746702 0.246186 0.727641
Hf 0.250000 0.750000 0.545455
Hf 0.249462 0.752035 0.636299
Hf 0.246815 0.746125 0.727647
Hf 0.250000 0.250000 0.545455
Hf 0.252206 0.249264 0.636307
Hf 0.246693 0.246229 0.727644
Hf 0.750000 0.750000 0.454545
Hf 0.752155 0.749302 0.363701
Hf 0.746753 0.746352 0.272343
Hf 0.750000 0.250000 0.454545
Hf 0.749390 0.252031 0.363694
Hf 0.746702 0.246186 0.272359
Hf 0.250000 0.750000 0.454545
Hf 0.249462 0.752035 0.363701
Hf 0.246815 0.746125 0.272353
Hf 0.250000 0.250000 0.454545
Hf 0.252206 0.249264 0.363693
Hf 0.246693 0.246229 0.272356
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.500000 0.750000 0.545455
O 0.500485 0.705403 0.637678
O 0.500701 0.796519 0.722634
O 0.500000 0.250000 0.545455
O 0.500237 0.299704 0.634515
O 0.499698 0.203092 0.731302
O 0.000000 0.750000 0.545455
O 0.000261 0.799612 0.634573
O 0.999758 0.702953 0.731135
O 0.000000 0.250000 0.545455
O 0.000470 0.205460 0.637746
O 0.000646 0.296370 0.722541
O 0.750000 0.750000 0.590909
O 0.768869 0.728215 0.681618
O 0.735181 0.794060 0.771591
O 0.750000 0.250000 0.590909
O 0.729343 0.270250 0.681628
O 0.794212 0.234083 0.771581
O 0.250000 0.750000 0.590909
O 0.230176 0.770347 0.681625
O 0.293974 0.733761 0.771590
O 0.250000 0.250000 0.590909
O 0.269550 0.227998 0.681622

O 0.234497 0.293810 0.771580
O 0.750000 0.500000 0.545455
O 0.799778 0.500139 0.634444
O 0.703823 0.499256 0.731381
O 0.750000 0.000000 0.545455
O 0.705533 0.000374 0.637781
O 0.797065 0.000188 0.722491
O 0.250000 0.500000 0.545455
O 0.205563 0.500359 0.637815
O 0.297083 0.500078 0.722495
O 0.250000 0.000000 0.545455
O 0.299737 0.000133 0.634421
O 0.203732 0.999159 0.731369
O 0.500000 0.750000 0.454545
O 0.500485 0.705403 0.362322
O 0.500701 0.796519 0.277366
O 0.500000 0.250000 0.454545
O 0.500237 0.299704 0.365485
O 0.499698 0.203092 0.268698
O 0.000000 0.750000 0.454545
O 0.000261 0.799612 0.365427
O 0.999758 0.702953 0.268865
O 0.000000 0.250000 0.454545
O 0.000470 0.205460 0.362254
O 0.000646 0.296370 0.277459
O 0.750000 0.750000 0.409091
O 0.768869 0.728215 0.318382
O 0.735181 0.794060 0.228409
O 0.750000 0.250000 0.409091
O 0.729343 0.270250 0.318372
O 0.794212 0.234083 0.228419
O 0.250000 0.750000 0.409091
O 0.230176 0.770347 0.318375
O 0.293974 0.733761 0.228410
O 0.250000 0.250000 0.409091
O 0.269550 0.227998 0.318378
O 0.234497 0.293810 0.228420
O 0.750000 0.500000 0.454545
O 0.799778 0.500139 0.365556
O 0.703823 0.499256 0.268619
O 0.750000 0.000000 0.454545
O 0.705533 0.000374 0.362219
O 0.797065 0.000188 0.277509
O 0.250000 0.500000 0.454545
O 0.205563 0.500359 0.362185
O 0.297083 0.500078 0.277505

O 0.250000 0.000000 0.454545
O 0.299737 0.000133 0.365579
O 0.203732 0.999159 0.268631

Structure 8. SrO-terminated $SrHfO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
_atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.060407  0.508983  0.774546
  Sr  0.511355  0.487681  0.773020
  Sr  0.972755  0.017601  0.767632
  Sr  0.487616  0.015430  0.766816
  Sr  0.500000  0.000000  0.500000
  Sr  0.000000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.000000  0.500000  0.500000
  Sr  0.000000  0.500000  0.590909
  Sr  0.007771  0.497052  0.682679
  Sr  0.500000  0.500000  0.590909
  Sr  0.508485  0.495875  0.681855
  Sr  0.000000  0.000000  0.590909
  Sr  0.000767  0.002255  0.679517
  Sr  0.500000  0.000000  0.590909
  Sr  0.487364  0.004655  0.679986
  Sr  0.060407  0.508983  0.225454
  Sr  0.511355  0.487681  0.226980
  Sr  0.972755  0.017601  0.232368
  Sr  0.487616  0.015430  0.233184
  Sr  0.000000  0.500000  0.409091
  Sr  0.007771  0.497052  0.317321
  Sr  0.500000  0.500000  0.409091
  Sr  0.508485  0.495875  0.318145
  Sr  0.000000  0.000000  0.409091
  Sr  0.000767  0.002255  0.320483
  Sr  0.500000  0.000000  0.409091
  Sr  0.487364  0.004655  0.320014
  Hf  0.249505  0.254644  0.727560
  Hf  0.748519  0.255270  0.727792
  Hf  0.254314  0.750685  0.728391
  Hf  0.750831  0.751531  0.724828
  Hf  0.250000  0.250000  0.545455
```

Hf 0.248002 0.248332 0.636221
Hf 0.750000 0.250000 0.545455
Hf 0.752636 0.252107 0.636426
Hf 0.250000 0.750000 0.545455
Hf 0.248674 0.751810 0.636621
Hf 0.750000 0.750000 0.545455
Hf 0.752526 0.747792 0.635841
Hf 0.249505 0.254644 0.272440
Hf 0.748519 0.255270 0.272208
Hf 0.254314 0.750685 0.271609
Hf 0.750831 0.751531 0.275172
Hf 0.250000 0.250000 0.454545
Hf 0.248002 0.248332 0.363779
Hf 0.750000 0.250000 0.454545
Hf 0.752636 0.252107 0.363574
Hf 0.250000 0.750000 0.454545
Hf 0.248674 0.751810 0.363379
Hf 0.750000 0.750000 0.454545
Hf 0.752526 0.747792 0.364159
C 0.805828 0.717744 0.794062
C 0.805828 0.717744 0.205938
O 0.275030 0.501232 0.718943
O 0.700697 0.505010 0.730023
O 0.217409 0.001665 0.733873
O 0.795473 0.999214 0.722330
O 0.717612 0.204832 0.770430
O 0.294724 0.698957 0.770728
O 0.999060 0.291565 0.732293
O 0.498136 0.213854 0.721563
O 0.996913 0.716064 0.733954
O 0.503866 0.799494 0.722570
O 0.281754 0.285020 0.771747
O 0.710892 0.796425 0.774670
O 0.770104 0.571493 0.800677
O 0.934889 0.786911 0.803057
O 0.750000 0.750000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.250000 0.250000 0.500000
O 0.250000 0.500000 0.545455
O 0.205956 0.499865 0.638081
O 0.750000 0.500000 0.545455
O 0.796714 0.500346 0.633674
O 0.250000 0.000000 0.545455
O 0.299826 0.999990 0.633954
O 0.750000 0.000000 0.545455

O 0.706900 0.999223 0.638644
O 0.250000 0.250000 0.590909
O 0.225975 0.221563 0.681410
O 0.750000 0.250000 0.590909
O 0.770921 0.275328 0.681473
O 0.250000 0.750000 0.590909
O 0.228743 0.778718 0.681727
O 0.750000 0.750000 0.590909
O 0.774676 0.723245 0.681670
O 0.000000 0.250000 0.545455
O 0.999753 0.201412 0.634101
O 0.500000 0.250000 0.545455
O 0.499701 0.293333 0.638095
O 0.000000 0.750000 0.545455
O 0.999751 0.798493 0.634340
O 0.500000 0.750000 0.545455
O 0.500849 0.705263 0.638210
O 0.275030 0.501232 0.281057
O 0.700697 0.505010 0.269977
O 0.217409 0.001665 0.266127
O 0.795473 0.999214 0.277670
O 0.717612 0.204832 0.229570
O 0.294724 0.698957 0.229272
O 0.999060 0.291565 0.267707
O 0.498136 0.213854 0.278437
O 0.996913 0.716064 0.266046
O 0.503866 0.799494 0.277430
O 0.281754 0.285020 0.228253
O 0.710892 0.796425 0.225330
O 0.770104 0.571493 0.199323
O 0.934889 0.786911 0.196943
O 0.250000 0.500000 0.454545
O 0.205956 0.499865 0.361919
O 0.750000 0.500000 0.454545
O 0.796714 0.500346 0.366326
O 0.250000 0.000000 0.454545
O 0.299826 0.999990 0.366046
O 0.750000 0.000000 0.454545
O 0.706900 0.999223 0.361356
O 0.250000 0.250000 0.409091
O 0.225975 0.221563 0.318590
O 0.750000 0.250000 0.409091
O 0.770921 0.275328 0.318527
O 0.250000 0.750000 0.409091
O 0.228743 0.778718 0.318273
O 0.750000 0.750000 0.409091

O 0.774676 0.723245 0.318330
O 0.000000 0.250000 0.454545
O 0.999753 0.201412 0.365899
O 0.500000 0.250000 0.454545
O 0.499701 0.293333 0.361905
O 0.000000 0.750000 0.454545
O 0.999751 0.798493 0.365660
O 0.500000 0.750000 0.454545
O 0.500849 0.705263 0.361790

Structure 9. SrO-terminated $SrHfO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.487469  0.548858  0.223367
  Sr  0.503946  0.022376  0.226542
  Sr  0.970930  0.462635  0.227991
  Sr  0.993480  0.992132  0.231467
  Sr  0.497591  0.504559  0.316649
  Sr  0.500267  0.010658  0.317448
  Sr  0.000134  0.989868  0.319877
  Sr  0.001300  0.494139  0.320701
  Sr  0.500000  0.500000  0.409091
  Sr  0.500000  0.000000  0.409091
  Sr  0.000000  0.000000  0.409091
  Sr  0.000000  0.500000  0.409091
  Sr  0.000000  0.000000  0.500000
  Sr  0.000000  0.500000  0.500000
  Sr  0.500000  0.000000  0.500000
  Sr  0.500000  0.500000  0.500000
  Sr  0.500000  0.500000  0.590909
  Sr  0.500000  0.000000  0.590909
  Sr  0.000000  0.500000  0.590909
  Sr  0.000000  0.000000  0.590909
  Sr  0.001300  0.494139  0.679299
  Sr  0.000134  0.989868  0.680123
  Sr  0.500267  0.010658  0.682552
  Sr  0.497591  0.504559  0.683351
  Sr  0.993480  0.992132  0.768533
  Sr  0.970930  0.462635  0.772008
  Sr  0.503946  0.022376  0.773458
  Sr  0.487469  0.548858  0.776633
  Hf  0.249707  0.751817  0.270847
  Hf  0.745476  0.248590  0.272150
  Hf  0.246012  0.251971  0.275020
  Hf  0.749342  0.747605  0.275194
  Hf  0.248296  0.748448  0.363154
```

Hf 0.747355 0.252412 0.363448
Hf 0.752343 0.747559 0.364108
Hf 0.252545 0.251879 0.364282
Hf 0.750000 0.750000 0.454545
Hf 0.750000 0.250000 0.454545
Hf 0.250000 0.750000 0.454545
Hf 0.250000 0.250000 0.454545
Hf 0.750000 0.750000 0.545455
Hf 0.750000 0.250000 0.545455
Hf 0.250000 0.750000 0.545455
Hf 0.250000 0.250000 0.545455
Hf 0.252545 0.251879 0.635718
Hf 0.752343 0.747559 0.635892
Hf 0.747355 0.252412 0.636552
Hf 0.248296 0.748448 0.636846
Hf 0.749342 0.747605 0.724806
Hf 0.246012 0.251971 0.724980
Hf 0.745476 0.248590 0.727850
Hf 0.249707 0.751817 0.729153
C 0.789515 0.732186 0.202807
C 0.282585 0.302947 0.205103
C 0.282585 0.302947 0.794897
C 0.789515 0.732186 0.797193
O 0.901429 0.813283 0.191345
O 0.749993 0.587204 0.195820
O 0.216426 0.434382 0.196990
O 0.425230 0.262230 0.197403
O 0.205871 0.210584 0.225379
O 0.706337 0.797521 0.226088
O 0.311846 0.793390 0.229732
O 0.789995 0.211001 0.230044
O 0.995200 0.720653 0.263594
O 0.711158 0.501812 0.267018
O 0.285569 0.497100 0.267534
O 0.494251 0.205317 0.270146
O 0.206371 0.003073 0.277615
O 0.999685 0.291794 0.277651
O 0.781863 0.995718 0.279267
O 0.502905 0.773664 0.281520
O 0.218633 0.729444 0.318189
O 0.786604 0.720884 0.318461
O 0.273593 0.272968 0.318487
O 0.724383 0.274165 0.318655
O 0.000660 0.207658 0.361347
O 0.501105 0.705861 0.361483
O 0.707027 0.998849 0.361541

O 0.294453 0.000627 0.361904
O 0.202439 0.499583 0.365688
O 0.799120 0.499936 0.366179
O 0.999968 0.800343 0.366211
O 0.499401 0.296180 0.366390
O 0.750000 0.750000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.250000 0.409091
O 0.250000 0.750000 0.409091
O 0.000000 0.750000 0.454545
O 0.000000 0.250000 0.454545
O 0.500000 0.250000 0.454545
O 0.500000 0.750000 0.454545
O 0.750000 0.500000 0.454545
O 0.750000 0.000000 0.454545
O 0.250000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.500000 0.750000 0.545455
O 0.500000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.000000 0.250000 0.545455
O 0.750000 0.500000 0.545455
O 0.750000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.250000 0.000000 0.545455
O 0.750000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.250000 0.250000 0.590909
O 0.499401 0.296180 0.633610
O 0.999968 0.800343 0.633789
O 0.799120 0.499936 0.633821
O 0.202439 0.499583 0.634312
O 0.294453 0.000627 0.638096
O 0.707027 0.998849 0.638459
O 0.501105 0.705861 0.638517
O 0.000660 0.207658 0.638653
O 0.724383 0.274165 0.681345
O 0.273593 0.272968 0.681513
O 0.786604 0.720884 0.681539
O 0.218633 0.729444 0.681811
O 0.502905 0.773664 0.718480

O 0.781863 0.995718 0.720733
O 0.999685 0.291794 0.722349
O 0.206371 0.003073 0.722385
O 0.494251 0.205317 0.729854
O 0.285569 0.497100 0.732466
O 0.711158 0.501812 0.732982
O 0.995200 0.720653 0.736406
O 0.789995 0.211001 0.769956
O 0.311846 0.793390 0.770268
O 0.706337 0.797521 0.773912
O 0.205871 0.210584 0.774621
O 0.425230 0.262230 0.802597
O 0.216426 0.434382 0.803010
O 0.749993 0.587204 0.804180
O 0.901429 0.813283 0.808655

Structure 10. BaO-terminated $BaTiO_3$ slab at Θ=0.00 CO_2 coverage

_cell_length_a 8.07335600
_cell_length_b 8.07335600
_cell_length_c 44.40346100
_cell_angle_alpha 90.00000000
_cell_angle_beta 90.00000000
_cell_angle_gamma 90.00000000
_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Ba 0.000000 0.000000 0.500000
Ba 0.000000 0.000000 0.590909
Ba 0.001708 0.996694 0.681867
Ba 0.000233 0.996620 0.771461
Ba 0.000000 0.500000 0.500000
Ba 0.000000 0.500000 0.590909
Ba 0.001250 0.497026 0.681845
Ba 0.998711 0.496738 0.771474
Ba 0.500000 0.000000 0.500000
Ba 0.500000 0.000000 0.590909
Ba 0.501717 0.996723 0.681849
Ba 0.500129 0.996622 0.771462
Ba 0.500000 0.500000 0.500000
Ba 0.500000 0.500000 0.590909
Ba 0.501331 0.497004 0.681825
Ba 0.498617 0.496728 0.771475
Ba 0.498617 0.496728 0.228525
Ba 0.501331 0.497004 0.318175
Ba 0.500000 0.500000 0.409091
Ba 0.500129 0.996622 0.228538
Ba 0.501717 0.996723 0.318151
Ba 0.500000 0.000000 0.409091
Ba 0.998711 0.496738 0.228526
Ba 0.001250 0.497026 0.318155
Ba 0.000000 0.500000 0.409091
Ba 0.000233 0.996620 0.228539
Ba 0.001708 0.996694 0.318133
Ba 0.000000 0.000000 0.409091
Ti 0.250000 0.250000 0.545455
Ti 0.259551 0.239921 0.636913
Ti 0.255841 0.241878 0.729152
Ti 0.250000 0.750000 0.545455

Ti 0.259839 0.739943 0.636901
Ti 0.245406 0.741847 0.729200
Ti 0.750000 0.250000 0.545455
Ti 0.759585 0.239925 0.636921
Ti 0.755816 0.241870 0.729175
Ti 0.750000 0.750000 0.545455
Ti 0.759852 0.739958 0.636909
Ti 0.745385 0.741845 0.729217
Ti 0.745385 0.741845 0.270783
Ti 0.759852 0.739958 0.363091
Ti 0.750000 0.750000 0.454545
Ti 0.755816 0.241870 0.270825
Ti 0.759585 0.239925 0.363079
Ti 0.750000 0.250000 0.454545
Ti 0.245406 0.741847 0.270800
Ti 0.259839 0.739943 0.363099
Ti 0.250000 0.750000 0.454545
Ti 0.255841 0.241878 0.270848
Ti 0.259551 0.239921 0.363087
Ti 0.250000 0.250000 0.454545
O 0.250000 0.000000 0.545455
O 0.246202 0.007700 0.636812
O 0.248710 0.005889 0.728778
O 0.250000 0.500000 0.545455
O 0.246229 0.507767 0.636813
O 0.248628 0.506010 0.728766
O 0.750000 0.000000 0.545455
O 0.746191 0.007693 0.636807
O 0.748738 0.005877 0.728785
O 0.750000 0.500000 0.545455
O 0.746233 0.507745 0.636808
O 0.748610 0.506010 0.728774
O 0.250000 0.250000 0.500000
O 0.250000 0.250000 0.590909
O 0.246778 0.253028 0.682254
O 0.246421 0.253785 0.772492
O 0.250000 0.750000 0.500000
O 0.250000 0.750000 0.590909
O 0.248538 0.753037 0.682245
O 0.250221 0.753624 0.772521
O 0.750000 0.250000 0.500000
O 0.750000 0.250000 0.590909
O 0.746755 0.253034 0.682236
O 0.746451 0.253776 0.772498
O 0.750000 0.750000 0.500000
O 0.750000 0.750000 0.590909

O 0.748557 0.753020 0.682225
O 0.750189 0.753624 0.772522
O 0.000000 0.250000 0.545455
O 0.992086 0.253620 0.636805
O 0.994827 0.253000 0.728777
O 0.000000 0.750000 0.545455
O 0.992554 0.753601 0.636783
O 0.001109 0.752883 0.728818
O 0.500000 0.250000 0.545455
O 0.492023 0.253621 0.636803
O 0.494866 0.252976 0.728781
O 0.500000 0.750000 0.545455
O 0.492522 0.753594 0.636784
O 0.501126 0.752910 0.728814
O 0.501126 0.752910 0.271186
O 0.492522 0.753594 0.363216
O 0.500000 0.750000 0.454545
O 0.494866 0.252976 0.271219
O 0.492023 0.253621 0.363197
O 0.500000 0.250000 0.454545
O 0.001109 0.752883 0.271182
O 0.992554 0.753601 0.363217
O 0.000000 0.750000 0.454545
O 0.994827 0.253000 0.271223
O 0.992086 0.253620 0.363195
O 0.000000 0.250000 0.454545
O 0.750189 0.753624 0.227478
O 0.748557 0.753020 0.317775
O 0.750000 0.750000 0.409091
O 0.746451 0.253776 0.227502
O 0.746755 0.253034 0.317764
O 0.750000 0.250000 0.409091
O 0.250221 0.753624 0.227479
O 0.248538 0.753037 0.317755
O 0.250000 0.750000 0.409091
O 0.246421 0.253785 0.227508
O 0.246778 0.253028 0.317746
O 0.250000 0.250000 0.409091
O 0.748610 0.506010 0.271226
O 0.746233 0.507745 0.363192
O 0.750000 0.500000 0.454545
O 0.748738 0.005877 0.271215
O 0.746191 0.007693 0.363193
O 0.750000 0.000000 0.454545
O 0.248628 0.506010 0.271234
O 0.246229 0.507767 0.363187

O 0.250000 0.500000 0.454545
O 0.248710 0.005889 0.271222
O 0.246202 0.007700 0.363188
O 0.250000 0.000000 0.454545

Structure 11. BaO-terminated $BaTiO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.07335600
_cell_length_b   8.07335600
_cell_length_c   44.40346100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.000000  0.500000  0.500000
  Ba  0.000000  0.500000  0.590909
  Ba  0.006546  0.500191  0.682518
  Ba  0.013002  0.493897  0.775977
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.000000  0.590909
  Ba  0.006029  0.006035  0.682421
  Ba  0.998907  0.996853  0.774923
  Ba  0.500000  0.500000  0.500000
  Ba  0.500000  0.500000  0.590909
  Ba  0.499357  0.499371  0.682573
  Ba  0.506804  0.503125  0.776005
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.499654  0.006977  0.682398
  Ba  0.494286  0.011085  0.773640
  Ba  0.494286  0.011085  0.226360
  Ba  0.499654  0.006977  0.317602
  Ba  0.500000  0.000000  0.409091
  Ba  0.506804  0.503125  0.223995
  Ba  0.499357  0.499371  0.317427
  Ba  0.500000  0.500000  0.409091
  Ba  0.998907  0.996853  0.225077
  Ba  0.006029  0.006035  0.317579
  Ba  0.000000  0.000000  0.409091
  Ba  0.013002  0.493897  0.224022
  Ba  0.006546  0.500191  0.317482
  Ba  0.000000  0.500000  0.409091
  Ti  0.250000  0.250000  0.545455
  Ti  0.259705  0.259747  0.636998
  Ti  0.257313  0.260069  0.730189
  Ti  0.250000  0.750000  0.545455
  Ti  0.261156  0.759576  0.637789
```

Ti 0.259772 0.755772 0.731357
Ti 0.750000 0.250000 0.545455
Ti 0.759328 0.261683 0.637783
Ti 0.758803 0.258994 0.731267
Ti 0.750000 0.750000 0.545455
Ti 0.759453 0.759080 0.634421
Ti 0.753992 0.755717 0.724352
Ti 0.753992 0.755717 0.275648
Ti 0.759453 0.759080 0.365579
Ti 0.750000 0.750000 0.454545
Ti 0.758803 0.258994 0.268733
Ti 0.759328 0.261683 0.362217
Ti 0.750000 0.250000 0.454545
Ti 0.259772 0.755772 0.268643
Ti 0.261156 0.759576 0.362211
Ti 0.250000 0.750000 0.454545
Ti 0.257313 0.260069 0.269811
Ti 0.259705 0.259747 0.363002
Ti 0.250000 0.250000 0.454545
C 0.795818 0.705538 0.810114
C 0.795818 0.705538 0.189886
O 0.711820 0.786076 0.788471
O 0.741402 0.563113 0.818534
O 0.935983 0.764726 0.818498
O 0.711820 0.786076 0.211529
O 0.741402 0.563113 0.181466
O 0.935983 0.764726 0.181502
O 0.250000 0.500000 0.545455
O 0.246627 0.492728 0.636742
O 0.245983 0.494818 0.728415
O 0.250000 0.000000 0.545455
O 0.246656 0.992533 0.636684
O 0.247170 0.991748 0.729126
O 0.750000 0.500000 0.545455
O 0.746031 0.495575 0.636940
O 0.745538 0.500849 0.732015
O 0.750000 0.000000 0.545455
O 0.746065 0.989593 0.637042
O 0.745053 0.988770 0.729924
O 0.250000 0.250000 0.500000
O 0.250000 0.250000 0.590909
O 0.247482 0.246893 0.681742
O 0.244971 0.249750 0.772761
O 0.250000 0.750000 0.500000
O 0.250000 0.750000 0.590909
O 0.246185 0.746933 0.681514

O 0.255498 0.743393 0.772462
O 0.750000 0.250000 0.500000
O 0.750000 0.250000 0.590909
O 0.746042 0.249271 0.681597
O 0.747285 0.239575 0.772279
O 0.750000 0.750000 0.500000
O 0.750000 0.750000 0.590909
O 0.750934 0.746168 0.683761
O 0.000000 0.250000 0.545455
O 0.992245 0.246819 0.636815
O 0.992879 0.248859 0.728510
O 0.000000 0.750000 0.545455
O 0.989846 0.746132 0.636764
O 0.986532 0.744615 0.732238
O 0.500000 0.250000 0.545455
O 0.492807 0.246708 0.636648
O 0.493111 0.247874 0.728901
O 0.500000 0.750000 0.545455
O 0.495382 0.746202 0.637190
O 0.500900 0.745586 0.730098
O 0.500900 0.745586 0.269902
O 0.495382 0.746202 0.362810
O 0.500000 0.750000 0.454545
O 0.493111 0.247874 0.271099
O 0.492807 0.246708 0.363352
O 0.500000 0.250000 0.454545
O 0.986532 0.744615 0.267762
O 0.989846 0.746132 0.363236
O 0.000000 0.750000 0.454545
O 0.992879 0.248859 0.271490
O 0.992245 0.246819 0.363185
O 0.000000 0.250000 0.454545
O 0.750934 0.746168 0.316239
O 0.750000 0.750000 0.409091
O 0.747285 0.239575 0.227721
O 0.746042 0.249271 0.318403
O 0.750000 0.250000 0.409091
O 0.255498 0.743393 0.227538
O 0.246185 0.746933 0.318486
O 0.250000 0.750000 0.409091
O 0.244971 0.249750 0.227239
O 0.247482 0.246893 0.318258
O 0.250000 0.250000 0.409091
O 0.745053 0.988770 0.270076
O 0.746065 0.989593 0.362958
O 0.750000 0.000000 0.454545

O 0.745538 0.500849 0.267985
O 0.746031 0.495575 0.363060
O 0.750000 0.500000 0.454545
O 0.247170 0.991748 0.270874
O 0.246656 0.992533 0.363316
O 0.250000 0.000000 0.454545
O 0.245983 0.494818 0.271585
O 0.246627 0.492728 0.363258
O 0.250000 0.500000 0.454545

Structure 12. BaO-terminated $BaTiO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.07335600
_cell_length_b   8.07335600
_cell_length_c   44.40346100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.502979  0.499342  0.777915
  Ba  0.499218  0.998860  0.777914
  Ba  0.000799  0.500082  0.777426
  Ba  0.000764  0.000385  0.777340
  Ba  0.498627  0.996760  0.683367
  Ba  0.499012  0.498078  0.683285
  Ba  0.999333  0.496718  0.683198
  Ba  0.998499  0.997610  0.683123
  Ba  0.000000  0.000000  0.590909
  Ba  0.000000  0.500000  0.590909
  Ba  0.500000  0.000000  0.590909
  Ba  0.500000  0.500000  0.590909
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.500000  0.500000
  Ba  0.500000  0.500000  0.500000
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.500000  0.409091
  Ba  0.500000  0.000000  0.409091
  Ba  0.000000  0.500000  0.409091
  Ba  0.000000  0.000000  0.409091
  Ba  0.998499  0.997610  0.316877
  Ba  0.999333  0.496718  0.316802
  Ba  0.499012  0.498078  0.316715
  Ba  0.498627  0.996760  0.316633
  Ba  0.000764  0.000385  0.222660
  Ba  0.000799  0.500082  0.222574
  Ba  0.499218  0.998860  0.222086
  Ba  0.502979  0.499342  0.222085
  Ti  0.257586  0.741982  0.732559
  Ti  0.742141  0.242074  0.732468
  Ti  0.244257  0.241983  0.726113
  Ti  0.756053  0.742087  0.726099
  Ti  0.739550  0.239457  0.638301
```

Ti 0.239669 0.739437 0.638281
Ti 0.241697 0.241213 0.634986
Ti 0.741591 0.741199 0.634961
Ti 0.750000 0.750000 0.545455
Ti 0.750000 0.250000 0.545455
Ti 0.250000 0.750000 0.545455
Ti 0.250000 0.250000 0.545455
Ti 0.250000 0.250000 0.454545
Ti 0.250000 0.750000 0.454545
Ti 0.750000 0.250000 0.454545
Ti 0.750000 0.750000 0.454545
Ti 0.741591 0.741199 0.365039
Ti 0.241697 0.241213 0.365014
Ti 0.239669 0.739437 0.361719
Ti 0.739550 0.239457 0.361699
Ti 0.756053 0.742087 0.273901
Ti 0.244257 0.241983 0.273887
Ti 0.742141 0.242074 0.267532
Ti 0.257586 0.741982 0.267441
C 0.751240 0.752535 0.807153
C 0.251193 0.252450 0.807060
C 0.251193 0.252450 0.192940
C 0.751240 0.752535 0.192847
O 0.749903 0.753876 0.776036
O 0.254136 0.254158 0.775950
O 0.249841 0.754620 0.773247
O 0.753334 0.254880 0.773178
O 0.501390 0.755708 0.730572
O 0.502323 0.255889 0.730505
O 0.008738 0.255796 0.730381
O 0.995005 0.755859 0.730373
O 0.251935 0.507941 0.729648
O 0.750754 0.007809 0.729641
O 0.251845 0.009303 0.729484
O 0.751015 0.509404 0.729440
O 0.751512 0.752575 0.684330
O 0.252214 0.252565 0.684320
O 0.753398 0.254122 0.680931
O 0.252315 0.754155 0.680895
O 0.754030 0.005288 0.637021
O 0.254090 0.505218 0.637013
O 0.505158 0.254148 0.637010
O 0.004869 0.754108 0.636966
O 0.510528 0.754225 0.636906
O 0.010729 0.254174 0.636895
O 0.754300 0.510723 0.636876

O 0.254331 0.010709 0.636859
O 0.750000 0.750000 0.590909
O 0.250000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.250000 0.250000 0.590909
O 0.750000 0.000000 0.545455
O 0.750000 0.500000 0.545455
O 0.250000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.000000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.500000 0.250000 0.545455
O 0.500000 0.750000 0.545455
O 0.750000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.250000 0.250000 0.500000
O 0.500000 0.250000 0.454545
O 0.500000 0.750000 0.454545
O 0.000000 0.750000 0.454545
O 0.000000 0.250000 0.454545
O 0.250000 0.000000 0.454545
O 0.750000 0.500000 0.454545
O 0.750000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.250000 0.250000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.750000 0.409091
O 0.750000 0.750000 0.409091
O 0.254331 0.010709 0.363141
O 0.754300 0.510723 0.363124
O 0.010729 0.254174 0.363105
O 0.510528 0.754225 0.363094
O 0.004869 0.754108 0.363034
O 0.505158 0.254148 0.362990
O 0.254090 0.505218 0.362987
O 0.754030 0.005288 0.362979
O 0.252315 0.754155 0.319105
O 0.753398 0.254122 0.319069
O 0.252214 0.252565 0.315680
O 0.751512 0.752575 0.315670
O 0.751015 0.509404 0.270560
O 0.251845 0.009303 0.270516
O 0.750754 0.007809 0.270359
O 0.251935 0.507941 0.270352
O 0.995005 0.755859 0.269627

O 0.008738 0.255796 0.269619
O 0.502323 0.255889 0.269495
O 0.501390 0.755708 0.269428
O 0.753334 0.254880 0.226822
O 0.249841 0.754620 0.226753
O 0.254136 0.254158 0.224050
O 0.749903 0.753876 0.223964
O 0.249731 0.109366 0.180925
O 0.752086 0.609566 0.180784
O 0.250705 0.394305 0.180490
O 0.751033 0.894543 0.180454
O 0.751033 0.894543 0.819546
O 0.250705 0.394305 0.819510
O 0.752086 0.609566 0.819216
O 0.249731 0.109366 0.819075

Structure 13. BaO-terminated $BaZrO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.499630  0.000030  0.681044
  Ba  0.487829  0.000572  0.769982
  Ba  0.500000  0.500000  0.500000
  Ba  0.500000  0.500000  0.590909
  Ba  0.499884  0.500277  0.681039
  Ba  0.499101  0.512348  0.769988
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.000000  0.590909
  Ba  0.999886  0.000275  0.681038
  Ba  0.999101  0.012349  0.769988
  Ba  0.000000  0.500000  0.500000
  Ba  0.000000  0.500000  0.590909
  Ba  0.999631  0.500031  0.681044
  Ba  0.987830  0.500572  0.769982
  Ba  0.500000  0.000000  0.409091
  Ba  0.499630  0.000030  0.318956
  Ba  0.487829  0.000572  0.230018
  Ba  0.500000  0.500000  0.409091
  Ba  0.499884  0.500277  0.318961
  Ba  0.499101  0.512348  0.230012
  Ba  0.000000  0.000000  0.409091
  Ba  0.999886  0.000275  0.318962
  Ba  0.999101  0.012349  0.230012
  Ba  0.000000  0.500000  0.409091
  Ba  0.999631  0.500031  0.318956
  Ba  0.987830  0.500572  0.230018
  Zr  0.750000  0.250000  0.545455
  Zr  0.749500  0.249489  0.636561
  Zr  0.747803  0.251627  0.728504
  Zr  0.750000  0.750000  0.545455
  Zr  0.750541  0.750481  0.636562
```

Zr 0.748262 0.752058 0.728508
Zr 0.250000 0.250000 0.545455
Zr 0.250541 0.250480 0.636562
Zr 0.248261 0.252058 0.728508
Zr 0.250000 0.750000 0.545455
Zr 0.249502 0.749488 0.636561
Zr 0.247803 0.751627 0.728504
Zr 0.750000 0.250000 0.454545
Zr 0.749500 0.249489 0.363439
Zr 0.747803 0.251627 0.271496
Zr 0.750000 0.750000 0.454545
Zr 0.750541 0.750481 0.363438
Zr 0.748262 0.752058 0.271492
Zr 0.250000 0.250000 0.454545
Zr 0.250541 0.250480 0.363438
Zr 0.248261 0.252058 0.271492
Zr 0.250000 0.750000 0.454545
Zr 0.249502 0.749488 0.363439
Zr 0.247803 0.751627 0.271496
O 0.750000 0.000000 0.545455
O 0.761754 0.999886 0.635943
O 0.721537 0.000429 0.729452
O 0.750000 0.500000 0.545455
O 0.739082 0.499875 0.636924
O 0.777708 0.500174 0.726446
O 0.250000 0.000000 0.545455
O 0.239081 0.999874 0.636924
O 0.277708 0.000174 0.726446
O 0.250000 0.500000 0.545455
O 0.261754 0.499885 0.635943
O 0.221537 0.500429 0.729452
O 0.750000 0.250000 0.500000
O 0.750000 0.250000 0.590909
O 0.744239 0.244626 0.681948
O 0.767860 0.259071 0.772523
O 0.750000 0.750000 0.500000
O 0.750000 0.750000 0.590909
O 0.755528 0.755425 0.681948
O 0.740209 0.732517 0.772528
O 0.250000 0.250000 0.500000
O 0.250000 0.250000 0.590909
O 0.255528 0.255427 0.681948
O 0.240210 0.232516 0.772528
O 0.250000 0.750000 0.500000
O 0.250000 0.750000 0.590909
O 0.244237 0.744626 0.681948

O 0.267860 0.759072 0.772523
O 0.500000 0.250000 0.545455
O 0.500066 0.238122 0.635926
O 0.499436 0.278285 0.729511
O 0.500000 0.750000 0.545455
O 0.500073 0.760789 0.636948
O 0.499689 0.722161 0.726377
O 0.000000 0.250000 0.545455
O 0.000073 0.260789 0.636948
O 0.999689 0.222161 0.726377
O 0.000000 0.750000 0.545455
O 0.000067 0.738122 0.635926
O 0.999436 0.778285 0.729511
O 0.750000 0.000000 0.454545
O 0.761754 0.999886 0.364057
O 0.721537 0.000429 0.270548
O 0.750000 0.500000 0.454545
O 0.739082 0.499875 0.363076
O 0.777708 0.500174 0.273554
O 0.250000 0.000000 0.454545
O 0.239081 0.999874 0.363076
O 0.277708 0.000174 0.273554
O 0.250000 0.500000 0.454545
O 0.261754 0.499885 0.364057
O 0.221537 0.500429 0.270548
O 0.750000 0.250000 0.409091
O 0.744239 0.244626 0.318052
O 0.767860 0.259071 0.227477
O 0.750000 0.750000 0.409091
O 0.755528 0.755425 0.318052
O 0.740209 0.732517 0.227472
O 0.250000 0.250000 0.409091
O 0.255528 0.255427 0.318052
O 0.240210 0.232516 0.227472
O 0.250000 0.750000 0.409091
O 0.244237 0.744626 0.318052
O 0.267860 0.759072 0.227477
O 0.500000 0.250000 0.454545
O 0.500066 0.238122 0.364074
O 0.499436 0.278285 0.270489
O 0.500000 0.750000 0.454545
O 0.500073 0.760789 0.363052
O 0.499689 0.722161 0.273623
O 0.000000 0.250000 0.454545
O 0.000073 0.260789 0.363052
O 0.999689 0.222161 0.273623

O 0.000000 0.750000 0.454545
O 0.000067 0.738122 0.364074
O 0.999436 0.778285 0.270489

Structure 14. BaO-terminated $BaZrO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.024347  0.496789  0.226304
  Ba  0.002389  0.011395  0.227529
  Ba  0.498800  0.504631  0.228366
  Ba  0.497355  0.016792  0.229395
  Ba  0.003275  0.002844  0.318301
  Ba  0.497418  0.003868  0.318374
  Ba  0.004184  0.496092  0.318547
  Ba  0.496478  0.497134  0.318662
  Ba  0.500000  0.000000  0.409091
  Ba  0.500000  0.500000  0.409091
  Ba  0.000000  0.500000  0.409091
  Ba  0.000000  0.000000  0.409091
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.500000  0.500000
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.500000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.500000  0.500000  0.590909
  Ba  0.000000  0.000000  0.590909
  Ba  0.000000  0.500000  0.590909
  Ba  0.496478  0.497134  0.681338
  Ba  0.004184  0.496092  0.681453
  Ba  0.497418  0.003868  0.681626
  Ba  0.003275  0.002844  0.681699
  Ba  0.497355  0.016792  0.770605
  Ba  0.498800  0.504631  0.771634
  Ba  0.002389  0.011395  0.772471
  Ba  0.024347  0.496789  0.773696
  Zr  0.753209  0.252464  0.270649
  Zr  0.251671  0.750630  0.270799
  Zr  0.250492  0.252478  0.271762
  Zr  0.751062  0.751393  0.274398
  Zr  0.749732  0.250661  0.363107
```

Zr 0.249426 0.750511 0.363153
Zr 0.250642 0.249028 0.363691
Zr 0.751180 0.748696 0.364101
Zr 0.250000 0.250000 0.454545
Zr 0.250000 0.750000 0.454545
Zr 0.750000 0.250000 0.454545
Zr 0.750000 0.750000 0.454545
Zr 0.250000 0.250000 0.545455
Zr 0.250000 0.750000 0.545455
Zr 0.750000 0.250000 0.545455
Zr 0.750000 0.750000 0.545455
Zr 0.751180 0.748696 0.635899
Zr 0.250642 0.249028 0.636309
Zr 0.249426 0.750511 0.636847
Zr 0.749732 0.250661 0.636893
Zr 0.751062 0.751393 0.725602
Zr 0.250492 0.252478 0.728238
Zr 0.251671 0.750630 0.729201
Zr 0.753209 0.252464 0.729351
C 0.790187 0.711833 0.201878
C 0.790187 0.711833 0.798122
O 0.736689 0.579748 0.193065
O 0.920661 0.769852 0.193149
O 0.713606 0.785659 0.223307
O 0.244491 0.256649 0.227516
O 0.273220 0.730841 0.228087
O 0.754964 0.213291 0.228166
O 0.772093 0.503844 0.266610
O 0.997359 0.771311 0.268034
O 0.272134 0.000083 0.271358
O 0.500979 0.269931 0.271555
O 0.000999 0.230113 0.273961
O 0.504184 0.726799 0.274127
O 0.227463 0.499475 0.274286
O 0.727674 0.996083 0.274821
O 0.763212 0.735584 0.317547
O 0.746359 0.260985 0.318084
O 0.241204 0.754977 0.318184
O 0.255666 0.243887 0.318417
O 0.761770 0.998633 0.362364
O 0.501232 0.761164 0.362544
O 0.261685 0.499526 0.363126
O 0.000250 0.260858 0.363206
O 0.500221 0.237137 0.364124
O 0.237898 0.999678 0.364244
O 0.999520 0.737324 0.364415

O 0.737372 0.500309 0.364507
O 0.250000 0.250000 0.409091
O 0.250000 0.750000 0.409091
O 0.750000 0.750000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.750000 0.000000 0.454545
O 0.750000 0.500000 0.454545
O 0.000000 0.250000 0.454545
O 0.000000 0.750000 0.454545
O 0.500000 0.750000 0.454545
O 0.500000 0.250000 0.454545
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.250000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.750000 0.000000 0.545455
O 0.750000 0.500000 0.545455
O 0.500000 0.250000 0.545455
O 0.500000 0.750000 0.545455
O 0.000000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.250000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.750000 0.750000 0.590909
O 0.737372 0.500309 0.635493
O 0.999520 0.737324 0.635585
O 0.237898 0.999678 0.635756
O 0.500221 0.237137 0.635876
O 0.000250 0.260858 0.636794
O 0.261685 0.499526 0.636874
O 0.501232 0.761164 0.637456
O 0.761770 0.998633 0.637636
O 0.255666 0.243887 0.681583
O 0.241204 0.754977 0.681816
O 0.746359 0.260985 0.681916
O 0.763212 0.735584 0.682453
O 0.727674 0.996083 0.725179
O 0.227463 0.499475 0.725714
O 0.504184 0.726799 0.725873
O 0.000999 0.230113 0.726039
O 0.500979 0.269931 0.728445

O 0.272134 0.000083 0.728642
O 0.997359 0.771311 0.731966
O 0.772093 0.503844 0.733390
O 0.754964 0.213291 0.771834
O 0.273220 0.730841 0.771913
O 0.244491 0.256649 0.772484
O 0.713606 0.785659 0.776693
O 0.920661 0.769852 0.806851
O 0.736689 0.579748 0.806935

Structure 15. BaO-terminated $BaZrO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.993741  0.483549  0.224502
  Ba  0.492218  0.519362  0.225127
  Ba  0.993454  0.997285  0.227568
  Ba  0.492797  0.004722  0.228162
  Ba  0.999079  0.498820  0.317825
  Ba  0.998971  0.000543  0.318043
  Ba  0.499853  0.501933  0.318292
  Ba  0.498910  0.999886  0.318293
  Ba  0.000000  0.000000  0.409091
  Ba  0.500000  0.000000  0.409091
  Ba  0.500000  0.500000  0.409091
  Ba  0.000000  0.500000  0.409091
  Ba  0.500000  0.000000  0.500000
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.500000  0.500000
  Ba  0.500000  0.500000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.000000  0.000000  0.590909
  Ba  0.000000  0.500000  0.590909
  Ba  0.500000  0.500000  0.590909
  Ba  0.498910  0.999886  0.681707
  Ba  0.499853  0.501933  0.681708
  Ba  0.998971  0.000543  0.681957
  Ba  0.999079  0.498820  0.682175
  Ba  0.492797  0.004722  0.771838
  Ba  0.993454  0.997285  0.772432
  Ba  0.492218  0.519362  0.774873
  Ba  0.993741  0.483549  0.775498
  Zr  0.748362  0.252006  0.270378
  Zr  0.247792  0.749924  0.270535
  Zr  0.247947  0.251153  0.274563
  Zr  0.747459  0.750972  0.274567
  Zr  0.748660  0.250432  0.362970
```

Zr 0.248498 0.749592 0.363004
Zr 0.251243 0.250766 0.364219
Zr 0.751262 0.749766 0.364249
Zr 0.750000 0.750000 0.454545
Zr 0.250000 0.750000 0.454545
Zr 0.250000 0.250000 0.454545
Zr 0.750000 0.250000 0.454545
Zr 0.750000 0.250000 0.545455
Zr 0.250000 0.250000 0.545455
Zr 0.250000 0.750000 0.545455
Zr 0.750000 0.750000 0.545455
Zr 0.751262 0.749766 0.635751
Zr 0.251243 0.250766 0.635782
Zr 0.248498 0.749592 0.636996
Zr 0.748660 0.250432 0.637030
Zr 0.747459 0.750972 0.725433
Zr 0.247947 0.251153 0.725437
Zr 0.247792 0.749924 0.729465
Zr 0.748362 0.252006 0.729622
C 0.286217 0.283111 0.200301
C 0.784565 0.716639 0.200337
C 0.784565 0.716639 0.799663
C 0.286217 0.283111 0.799699
O 0.404550 0.212471 0.190040
O 0.905793 0.783989 0.190340
O 0.730979 0.585539 0.191326
O 0.235783 0.416122 0.191521
O 0.215996 0.221989 0.224195
O 0.715732 0.779079 0.224215
O 0.787993 0.235350 0.228735
O 0.284632 0.768167 0.228813
O 0.495472 0.261095 0.267493
O 0.995422 0.760758 0.268434
O 0.237145 0.497515 0.269750
O 0.757639 0.504526 0.270193
O 0.737862 0.998546 0.273901
O 0.258267 0.003644 0.274399
O 0.502111 0.738609 0.275989
O 0.002564 0.243553 0.276486
O 0.266428 0.259273 0.317997
O 0.764579 0.744895 0.318019
O 0.737164 0.255893 0.318292
O 0.238039 0.743588 0.318341
O 0.001018 0.260167 0.362294
O 0.500947 0.760771 0.362385
O 0.239314 0.001018 0.362937

O 0.760946 0.999286 0.363172
O 0.738947 0.500844 0.363970
O 0.261326 0.499443 0.364226
O 0.999392 0.739271 0.364899
O 0.499473 0.237819 0.364920
O 0.750000 0.750000 0.409091
O 0.250000 0.750000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.250000 0.409091
O 0.000000 0.250000 0.454545
O 0.500000 0.250000 0.454545
O 0.500000 0.750000 0.454545
O 0.750000 0.000000 0.454545
O 0.000000 0.750000 0.454545
O 0.250000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.750000 0.500000 0.454545
O 0.750000 0.750000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.250000 0.250000 0.500000
O 0.000000 0.750000 0.545455
O 0.500000 0.250000 0.545455
O 0.750000 0.000000 0.545455
O 0.000000 0.250000 0.545455
O 0.500000 0.750000 0.545455
O 0.250000 0.000000 0.545455
O 0.750000 0.500000 0.545455
O 0.250000 0.500000 0.545455
O 0.250000 0.750000 0.590909
O 0.750000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.250000 0.250000 0.590909
O 0.499473 0.237819 0.635080
O 0.999392 0.739271 0.635101
O 0.261326 0.499443 0.635774
O 0.738947 0.500844 0.636030
O 0.760946 0.999286 0.636828
O 0.239314 0.001018 0.637063
O 0.500947 0.760771 0.637615
O 0.001018 0.260167 0.637706
O 0.238039 0.743588 0.681659
O 0.737164 0.255893 0.681708
O 0.764579 0.744895 0.681981
O 0.266428 0.259273 0.682003
O 0.002564 0.243553 0.723514

O 0.502111 0.738609 0.724011
O 0.258267 0.003644 0.725601
O 0.737862 0.998546 0.726099
O 0.757639 0.504526 0.729807
O 0.237145 0.497515 0.730250
O 0.995422 0.760758 0.731566
O 0.495472 0.261095 0.732507
O 0.284632 0.768167 0.771187
O 0.787993 0.235350 0.771265
O 0.715732 0.779079 0.775784
O 0.215996 0.221989 0.775805
O 0.235783 0.416122 0.808479
O 0.730979 0.585539 0.808674
O 0.905793 0.783989 0.809660
O 0.404550 0.212471 0.809960

Structure 16. BaO-terminated $BaHfO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.41088800
_cell_length_b   8.41088800
_cell_length_c   46.25988800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.500783  0.000588  0.681397
  Ba  0.503298  0.003420  0.770275
  Ba  0.500000  0.500000  0.500000
  Ba  0.500000  0.500000  0.590909
  Ba  0.500329  0.500003  0.681383
  Ba  0.498273  0.497684  0.770276
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.000000  0.590909
  Ba  0.000422  0.000124  0.681381
  Ba  0.998590  0.997690  0.770293
  Ba  0.000000  0.500000  0.500000
  Ba  0.000000  0.500000  0.590909
  Ba  0.000732  0.500449  0.681391
  Ba  0.003001  0.503533  0.770322
  Ba  0.500000  0.000000  0.409091
  Ba  0.500783  0.000588  0.318603
  Ba  0.503298  0.003420  0.229725
  Ba  0.500000  0.500000  0.409091
  Ba  0.500329  0.500003  0.318617
  Ba  0.498273  0.497684  0.229724
  Ba  0.000000  0.000000  0.409091
  Ba  0.000422  0.000124  0.318619
  Ba  0.998590  0.997690  0.229707
  Ba  0.000000  0.500000  0.409091
  Ba  0.000732  0.500449  0.318609
  Ba  0.003001  0.503533  0.229678
  Hf  0.750000  0.750000  0.545455
  Hf  0.750098  0.749963  0.636592
  Hf  0.750698  0.750368  0.728531
  Hf  0.750000  0.250000  0.545455
  Hf  0.750556  0.250355  0.636587
```

Hf 0.750896 0.250572 0.728543
Hf 0.250000 0.750000 0.545455
Hf 0.250604 0.750346 0.636588
Hf 0.250852 0.750521 0.728527
Hf 0.250000 0.250000 0.545455
Hf 0.250136 0.249943 0.636582
Hf 0.250591 0.250345 0.728537
Hf 0.750000 0.750000 0.454545
Hf 0.750098 0.749963 0.363408
Hf 0.750698 0.750368 0.271469
Hf 0.750000 0.250000 0.454545
Hf 0.750556 0.250355 0.363413
Hf 0.750896 0.250572 0.271457
Hf 0.250000 0.750000 0.454545
Hf 0.250604 0.750346 0.363412
Hf 0.250852 0.750521 0.271473
Hf 0.250000 0.250000 0.454545
Hf 0.250136 0.249943 0.363418
Hf 0.250591 0.250345 0.271463
O 0.750000 0.000000 0.545455
O 0.751624 0.000156 0.636670
O 0.750685 0.000463 0.727445
O 0.750000 0.500000 0.545455
O 0.749311 0.500150 0.636349
O 0.750770 0.500459 0.728552
O 0.250000 0.000000 0.545455
O 0.249240 0.000134 0.636337
O 0.250846 0.000407 0.728538
O 0.250000 0.500000 0.545455
O 0.251571 0.500130 0.636670
O 0.250851 0.500404 0.727434
O 0.750000 0.750000 0.500000
O 0.750000 0.750000 0.590909
O 0.748259 0.748573 0.681946
O 0.757663 0.755764 0.772732
O 0.750000 0.250000 0.500000
O 0.750000 0.250000 0.590909
O 0.752286 0.252086 0.681944
O 0.744723 0.245256 0.772741
O 0.250000 0.750000 0.500000
O 0.250000 0.750000 0.590909
O 0.252889 0.752025 0.681943
O 0.244123 0.745075 0.772728
O 0.250000 0.250000 0.500000
O 0.250000 0.250000 0.590909
O 0.248738 0.248493 0.681939

O 0.256755 0.255654 0.772733
O 0.500000 0.750000 0.545455
O 0.500374 0.751280 0.636292
O 0.500788 0.750428 0.728721
O 0.500000 0.250000 0.545455
O 0.500364 0.248968 0.636660
O 0.500738 0.250424 0.727396
O 0.000000 0.750000 0.545455
O 0.000377 0.748979 0.636722
O 0.000787 0.750434 0.727266
O 0.000000 0.250000 0.545455
O 0.000361 0.251274 0.636338
O 0.000736 0.250376 0.728571
O 0.750000 0.000000 0.454545
O 0.751624 0.000156 0.363330
O 0.750685 0.000463 0.272555
O 0.750000 0.500000 0.454545
O 0.749311 0.500150 0.363651
O 0.750770 0.500459 0.271448
O 0.250000 0.000000 0.454545
O 0.249240 0.000134 0.363663
O 0.250846 0.000407 0.271462
O 0.250000 0.500000 0.454545
O 0.251571 0.500130 0.363330
O 0.250851 0.500404 0.272566
O 0.750000 0.750000 0.409091
O 0.748259 0.748573 0.318054
O 0.757663 0.755764 0.227268
O 0.750000 0.250000 0.409091
O 0.752286 0.252086 0.318056
O 0.744723 0.245256 0.227259
O 0.250000 0.750000 0.409091
O 0.252889 0.752025 0.318057
O 0.244123 0.745075 0.227272
O 0.250000 0.250000 0.409091
O 0.248738 0.248493 0.318061
O 0.256755 0.255654 0.227267
O 0.500000 0.750000 0.454545
O 0.500374 0.751280 0.363708
O 0.500788 0.750428 0.271279
O 0.500000 0.250000 0.454545
O 0.500364 0.248968 0.363340
O 0.500738 0.250424 0.272604
O 0.000000 0.750000 0.454545
O 0.000377 0.748979 0.363278
O 0.000787 0.750434 0.272734

O 0.000000 0.250000 0.454545
O 0.000361 0.251274 0.363662
O 0.000736 0.250376 0.271429

Structure 17. BaO-terminated $BaHfO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.41088800
_cell_length_b   8.41088800
_cell_length_c   46.25988800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.009914  0.481570  0.226426
  Ba  0.001604  0.004273  0.227512
  Ba  0.492414  0.498775  0.227556
  Ba  0.489124  0.007747  0.228894
  Ba  0.497870  0.001531  0.318264
  Ba  0.003404  0.496109  0.318291
  Ba  0.497382  0.497298  0.318296
  Ba  0.002543  0.002366  0.318339
  Ba  0.500000  0.000000  0.409091
  Ba  0.500000  0.500000  0.409091
  Ba  0.000000  0.500000  0.409091
  Ba  0.000000  0.000000  0.409091
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.500000  0.500000
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.500000  0.500000
  Ba  0.500000  0.000000  0.590909
  Ba  0.500000  0.500000  0.590909
  Ba  0.000000  0.000000  0.590909
  Ba  0.000000  0.500000  0.590909
  Ba  0.002543  0.002366  0.681661
  Ba  0.497382  0.497298  0.681704
  Ba  0.003404  0.496109  0.681709
  Ba  0.497870  0.001531  0.681736
  Ba  0.489124  0.007747  0.771106
  Ba  0.492414  0.498775  0.772444
  Ba  0.001604  0.004273  0.772488
  Ba  0.009914  0.481570  0.773574
  Hf  0.250033  0.748297  0.270896
  Hf  0.751022  0.248708  0.270910
  Hf  0.249317  0.249839  0.272046
  Hf  0.749890  0.749399  0.274214
  Hf  0.249508  0.749931  0.363216
```

Hf 0.749743 0.250226 0.363217
Hf 0.250752 0.249373 0.363709
Hf 0.751119 0.748904 0.364004
Hf 0.250000 0.250000 0.454545
Hf 0.250000 0.750000 0.454545
Hf 0.750000 0.250000 0.454545
Hf 0.750000 0.750000 0.454545
Hf 0.250000 0.250000 0.545455
Hf 0.250000 0.750000 0.545455
Hf 0.750000 0.250000 0.545455
Hf 0.750000 0.750000 0.545455
Hf 0.751119 0.748904 0.635996
Hf 0.250752 0.249373 0.636291
Hf 0.749743 0.250226 0.636783
Hf 0.249508 0.749931 0.636784
Hf 0.749890 0.749399 0.725786
Hf 0.249317 0.249839 0.727954
Hf 0.751022 0.248708 0.729090
Hf 0.250033 0.748297 0.729104
C 0.787702 0.709772 0.200547
C 0.787702 0.709772 0.799453
O 0.726171 0.581624 0.190786
O 0.917737 0.769028 0.191141
O 0.718778 0.778824 0.224012
O 0.244460 0.252008 0.227614
O 0.762581 0.228069 0.227962
O 0.277268 0.746391 0.228023
O 0.997178 0.748724 0.268258
O 0.750664 0.502350 0.268565
O 0.500254 0.248861 0.271661
O 0.250731 0.999523 0.272298
O 0.248501 0.498961 0.273221
O 0.750007 0.996129 0.273663
O 0.000858 0.251337 0.273932
O 0.503514 0.748996 0.274161
O 0.760385 0.740976 0.317664
O 0.242751 0.751179 0.318180
O 0.747026 0.255896 0.318180
O 0.254404 0.247749 0.318444
O 0.501115 0.749806 0.362743
O 0.750390 0.998794 0.362857
O 0.000367 0.249557 0.363311
O 0.250583 0.499592 0.363468
O 0.250240 0.999712 0.363847
O 0.500244 0.249346 0.364034
O 0.749924 0.500201 0.364051

O 0.999718 0.749771 0.364196
O 0.250000 0.250000 0.409091
O 0.250000 0.750000 0.409091
O 0.750000 0.750000 0.409091
O 0.750000 0.250000 0.409091
O 0.250000 0.000000 0.454545
O 0.250000 0.500000 0.454545
O 0.750000 0.000000 0.454545
O 0.750000 0.500000 0.454545
O 0.000000 0.250000 0.454545
O 0.000000 0.750000 0.454545
O 0.500000 0.750000 0.454545
O 0.500000 0.250000 0.454545
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.750000 0.750000 0.500000
O 0.250000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.750000 0.000000 0.545455
O 0.750000 0.500000 0.545455
O 0.500000 0.250000 0.545455
O 0.500000 0.750000 0.545455
O 0.000000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.250000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.750000 0.750000 0.590909
O 0.999718 0.749771 0.635804
O 0.749924 0.500201 0.635949
O 0.500244 0.249346 0.635966
O 0.250240 0.999712 0.636153
O 0.250583 0.499592 0.636532
O 0.000367 0.249557 0.636689
O 0.750390 0.998794 0.637143
O 0.501115 0.749806 0.637257
O 0.254404 0.247749 0.681556
O 0.242751 0.751179 0.681820
O 0.747026 0.255896 0.681820
O 0.760385 0.740976 0.682336
O 0.503514 0.748996 0.725839
O 0.000858 0.251337 0.726068
O 0.750007 0.996129 0.726337
O 0.248501 0.498961 0.726779
O 0.250731 0.999523 0.727702

O 0.500254 0.248861 0.728339
O 0.750664 0.502350 0.731435
O 0.997178 0.748724 0.731742
O 0.277268 0.746391 0.771977
O 0.762581 0.228069 0.772038
O 0.244460 0.252008 0.772386
O 0.718778 0.778824 0.775988
O 0.917737 0.769028 0.808859
O 0.726171 0.581624 0.809214

Structure 18. BaO-terminated $BaHfO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.41088800
_cell_length_b   8.41088800
_cell_length_c   46.25988800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.517434  0.015836  0.224657
  Ba  0.994848  0.491801  0.224695
  Ba  0.993913  0.008541  0.224813
  Ba  0.516338  0.483340  0.224922
  Ba  0.498214  0.998365  0.317897
  Ba  0.497896  0.501414  0.317913
  Ba  0.002708  0.502635  0.317933
  Ba  0.002509  0.997130  0.317934
  Ba  0.000000  0.000000  0.409091
  Ba  0.000000  0.500000  0.409091
  Ba  0.500000  0.500000  0.409091
  Ba  0.500000  0.000000  0.409091
  Ba  0.000000  0.000000  0.500000
  Ba  0.000000  0.500000  0.500000
  Ba  0.500000  0.000000  0.500000
  Ba  0.500000  0.500000  0.500000
  Ba  0.000000  0.000000  0.590909
  Ba  0.000000  0.500000  0.590909
  Ba  0.500000  0.000000  0.590909
  Ba  0.500000  0.500000  0.590909
  Ba  0.002509  0.997130  0.682066
  Ba  0.002708  0.502635  0.682067
  Ba  0.497896  0.501414  0.682087
  Ba  0.498214  0.998365  0.682103
  Ba  0.516338  0.483340  0.775078
  Ba  0.993913  0.008541  0.775187
  Ba  0.994848  0.491801  0.775305
  Ba  0.517434  0.015836  0.775343
  Hf  0.249067  0.749617  0.268975
  Hf  0.751680  0.249693  0.272184
  Hf  0.750762  0.749793  0.274463
  Hf  0.250876  0.250001  0.274492
  Hf  0.250920  0.750094  0.362932
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Hf 0.750621 0.250025 0.363311
Hf 0.749167 0.749800 0.364146
Hf 0.249618 0.249773 0.364173
Hf 0.250000 0.250000 0.454545
Hf 0.250000 0.750000 0.454545
Hf 0.750000 0.250000 0.454545
Hf 0.750000 0.750000 0.454545
Hf 0.250000 0.250000 0.545455
Hf 0.250000 0.750000 0.545455
Hf 0.750000 0.250000 0.545455
Hf 0.750000 0.750000 0.545455
Hf 0.249618 0.249773 0.635827
Hf 0.749167 0.749800 0.635854
Hf 0.750621 0.250025 0.636689
Hf 0.250920 0.750094 0.637068
Hf 0.250876 0.250001 0.725508
Hf 0.750762 0.749793 0.725537
Hf 0.751680 0.249693 0.727816
Hf 0.249067 0.749617 0.731025
C 0.252639 0.248644 0.197728
C 0.749664 0.748889 0.198216
C 0.749664 0.748889 0.801784
C 0.252639 0.248644 0.802272
O 0.386629 0.244820 0.185128
O 0.737047 0.883719 0.186057
O 0.113396 0.246371 0.186940
O 0.741180 0.610662 0.187111
O 0.220468 0.745740 0.226622
O 0.259067 0.256281 0.227427
O 0.776265 0.752704 0.227517
O 0.740359 0.247163 0.228830
O 0.502807 0.749673 0.268554
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O 0.002147 0.249675 0.271208
O 0.749742 0.501349 0.271974
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O 0.749786 0.998134 0.272624
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O 0.499438 0.250536 0.363266
O 0.249399 0.499361 0.363376

O 0.749487 0.999261 0.363553
O 0.250640 0.000461 0.363611
O 0.750773 0.500526 0.363717
O 0.000692 0.249284 0.364074
O 0.500402 0.749263 0.364259
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O 0.250000 0.750000 0.409091
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O 0.750000 0.250000 0.409091
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O 0.750000 0.500000 0.454545
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O 0.000000 0.750000 0.454545
O 0.500000 0.750000 0.454545
O 0.500000 0.250000 0.454545
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O 0.750000 0.750000 0.500000
O 0.250000 0.000000 0.545455
O 0.250000 0.500000 0.545455
O 0.750000 0.000000 0.545455
O 0.750000 0.500000 0.545455
O 0.000000 0.250000 0.545455
O 0.000000 0.750000 0.545455
O 0.500000 0.250000 0.545455
O 0.500000 0.750000 0.545455
O 0.250000 0.250000 0.590909
O 0.250000 0.750000 0.590909
O 0.750000 0.250000 0.590909
O 0.750000 0.750000 0.590909
O 0.500402 0.749263 0.635741
O 0.000692 0.249284 0.635926
O 0.750773 0.500526 0.636283
O 0.250640 0.000461 0.636389
O 0.749487 0.999261 0.636447
O 0.249399 0.499361 0.636624
O 0.499438 0.250536 0.636734
O 0.999319 0.750506 0.637160
O 0.753944 0.250688 0.681528
O 0.245986 0.248215 0.681812
O 0.739806 0.748761 0.681831
O 0.257551 0.751342 0.681972
O 0.997315 0.749954 0.725137

O 0.498828 0.249946 0.726565
O 0.749786 0.998134 0.727376
O 0.250253 0.497516 0.727714
O 0.749742 0.501349 0.728026
O 0.002147 0.249675 0.728792
O 0.249996 0.002526 0.728877
O 0.502807 0.749673 0.731446
O 0.740359 0.247163 0.771170
O 0.776265 0.752704 0.772483
O 0.259067 0.256281 0.772573
O 0.220468 0.745740 0.773378
O 0.741180 0.610662 0.812889
O 0.113396 0.246371 0.813060
O 0.737047 0.883719 0.813943
O 0.386629 0.244820 0.814872

Structure 19. TiO_2-terminated $SrTiO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   7.89043600
_cell_length_b   7.89043600
_cell_length_c   43.39739600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.000000  0.000000  0.545440
  Sr  0.000000  0.499857  0.545440
  Sr  0.499857  0.000000  0.545440
  Sr  0.499857  0.499857  0.545440
  Sr  0.496676  0.496653  0.636815
  Sr  0.496674  0.996620  0.636814
  Sr  0.996643  0.496651  0.636814
  Sr  0.996641  0.996618  0.636812
  Sr  0.494971  0.494821  0.730588
  Sr  0.494969  0.994774  0.730591
  Sr  0.994923  0.494819  0.730591
  Sr  0.994921  0.994771  0.730594
  Sr  0.000000  0.000000  0.454560
  Sr  0.000000  0.499857  0.454560
  Sr  0.499857  0.000000  0.454560
  Sr  0.499857  0.499857  0.454560
  Sr  0.496676  0.496653  0.363185
  Sr  0.496674  0.996620  0.363186
  Sr  0.996643  0.496651  0.363186
  Sr  0.996641  0.996618  0.363188
  Sr  0.494971  0.494821  0.269412
  Sr  0.494969  0.994774  0.269409
  Sr  0.994923  0.494819  0.269409
  Sr  0.994921  0.994771  0.269406
  Ti  0.249929  0.249929  0.499998
  Ti  0.249929  0.749786  0.499998
  Ti  0.749786  0.249929  0.499998
  Ti  0.749786  0.749786  0.499998
  Ti  0.249929  0.249929  0.590881
  Ti  0.249929  0.749786  0.590881
  Ti  0.749786  0.249929  0.590881
  Ti  0.749786  0.749786  0.590881
  Ti  0.242119  0.242051  0.681348
```

Ti 0.242130 0.742022 0.681354
Ti 0.742089 0.242062 0.681354
Ti 0.742100 0.742033 0.681360
Ti 0.241344 0.241067 0.770353
Ti 0.241352 0.741034 0.770356
Ti 0.741310 0.241075 0.770356
Ti 0.741318 0.741042 0.770358
Ti 0.249929 0.249929 0.409119
Ti 0.249929 0.749786 0.409119
Ti 0.749786 0.249929 0.409119
Ti 0.749786 0.749786 0.409119
Ti 0.242119 0.242051 0.318652
Ti 0.242130 0.742022 0.318646
Ti 0.742089 0.242062 0.318646
Ti 0.742100 0.742033 0.318640
Ti 0.241344 0.241067 0.229647
Ti 0.241352 0.741034 0.229644
Ti 0.741310 0.241075 0.229644
Ti 0.741318 0.741042 0.229642
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O 0.749786 0.000000 0.590881
O 0.749786 0.499857 0.590881
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O 0.000000 0.749786 0.590881
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O 0.499857 0.749786 0.590881
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O 0.251602 0.751362 0.636413
O 0.751491 0.251472 0.636413
O 0.751490 0.751360 0.636405
O 0.003539 0.253629 0.681753
O 0.003533 0.753521 0.681753
O 0.503526 0.253632 0.681754

O 0.503520 0.753524 0.681753
O 0.253066 0.252709 0.727543
O 0.253064 0.752596 0.727547
O 0.752952 0.252707 0.727547
O 0.752949 0.752594 0.727550
O 0.253899 0.003303 0.681754
O 0.253902 0.503290 0.681754
O 0.753789 0.003297 0.681753
O 0.753792 0.503284 0.681754
O 0.006863 0.255164 0.772575
O 0.006861 0.755056 0.772575
O 0.506843 0.255169 0.772581
O 0.506841 0.755061 0.772581
O 0.255568 0.006493 0.772595
O 0.255573 0.506472 0.772601
O 0.755461 0.006491 0.772595
O 0.755466 0.506470 0.772602
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O 0.249929 0.499857 0.409119
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O 0.749786 0.499857 0.409119
O 0.249929 0.249929 0.454560
O 0.249929 0.749786 0.454560
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O 0.749786 0.749786 0.454560
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O 0.000000 0.749786 0.409119
O 0.499857 0.249929 0.409119
O 0.499857 0.749786 0.409119
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O 0.251602 0.751362 0.363587
O 0.751491 0.251472 0.363587
O 0.751490 0.751360 0.363595
O 0.003539 0.253629 0.318247
O 0.003533 0.753521 0.318247
O 0.503526 0.253632 0.318246
O 0.503520 0.753524 0.318247
O 0.253066 0.252709 0.272457
O 0.253064 0.752596 0.272453
O 0.752952 0.252707 0.272453
O 0.752949 0.752594 0.272450
O 0.253899 0.003303 0.318246
O 0.253902 0.503290 0.318246
O 0.753789 0.003297 0.318247
O 0.753792 0.503284 0.318246
O 0.006863 0.255164 0.227425

O 0.006861 0.755056 0.227425
O 0.506843 0.255169 0.227419
O 0.506841 0.755061 0.227419
O 0.255568 0.006493 0.227405
O 0.255573 0.506472 0.227399
O 0.755461 0.006491 0.227405
O 0.755466 0.506470 0.227398

Structure 20. TiO_2-terminated $SrTiO_3$ slab at Θ=0.25 CO_2 coverage

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_cell_length_a   7.89043600
_cell_length_b   7.89043600
_cell_length_c   43.39739600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
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  Sr  0.496185  0.993802  0.270704
  Sr  0.995993  0.995825  0.271026
  Sr  0.997511  0.487600  0.271976
  Sr  0.497317  0.499474  0.363342
  Sr  0.997106  0.994193  0.363384
  Sr  0.997260  0.499103  0.363413
  Sr  0.497384  0.993837  0.363420
  Sr  0.000000  0.000000  0.454560
  Sr  0.000000  0.499857  0.454560
  Sr  0.499857  0.000000  0.454560
  Sr  0.499857  0.499857  0.454560
  Sr  0.000000  0.000000  0.545440
  Sr  0.000000  0.499857  0.545440
  Sr  0.499857  0.000000  0.545440
  Sr  0.499857  0.499857  0.545440
  Sr  0.497384  0.993837  0.636580
  Sr  0.997260  0.499103  0.636587
  Sr  0.997106  0.994193  0.636616
  Sr  0.497317  0.499474  0.636658
  Sr  0.997511  0.487600  0.728024
  Sr  0.995993  0.995825  0.728974
  Sr  0.496185  0.993802  0.729296
  Sr  0.496769  0.494562  0.729611
  Ti  0.770631  0.734773  0.226846
  Ti  0.232012  0.735810  0.226971
  Ti  0.740760  0.237827  0.230364
  Ti  0.241353  0.237416  0.230408
  Ti  0.743860  0.742153  0.317458
  Ti  0.243816  0.742195  0.317536
  Ti  0.742476  0.242261  0.319103
  Ti  0.244146  0.241982  0.319117
  Ti  0.249929  0.249929  0.409118
```

Ti 0.249929 0.749786 0.409118
Ti 0.749786 0.749786 0.409118
Ti 0.749786 0.249929 0.409118
Ti 0.249929 0.749786 0.499998
Ti 0.749786 0.249929 0.499998
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Ti 0.244146 0.241982 0.680883
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Ti 0.743860 0.742153 0.682542
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Ti 0.740760 0.237827 0.769636
Ti 0.232012 0.735810 0.773030
Ti 0.770631 0.734773 0.773154
C 0.501524 0.759491 0.196400
C 0.501524 0.759491 0.803600
O 0.647693 0.759734 0.184192
O 0.355308 0.759845 0.184260
O 0.001533 0.763311 0.225125
O 0.505027 0.260165 0.227540
O 0.501966 0.754518 0.227850
O 0.760503 0.506802 0.228097
O 0.245944 0.507577 0.228451
O 0.005115 0.252659 0.228870
O 0.254742 0.007403 0.229763
O 0.750223 0.007729 0.229981
O 0.753664 0.749734 0.271731
O 0.250238 0.751591 0.271766
O 0.748514 0.257802 0.273160
O 0.255756 0.256256 0.273160
O 0.502919 0.754233 0.317405
O 0.753775 0.003295 0.317860
O 0.003026 0.254072 0.317893
O 0.002897 0.752762 0.317937
O 0.252500 0.003221 0.318102
O 0.253823 0.503290 0.318376
O 0.752526 0.503144 0.318626
O 0.502637 0.252640 0.318880
O 0.750331 0.752258 0.363452
O 0.251997 0.751670 0.363452
O 0.250185 0.251244 0.363681

O 0.752572 0.250555 0.363689
O 0.249929 0.000000 0.409118
O 0.249929 0.499857 0.409118
O 0.749786 0.499857 0.409118
O 0.749786 0.000000 0.409118
O 0.000000 0.249929 0.409118
O 0.000000 0.749786 0.409118
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O 0.249929 0.749786 0.454560
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O 0.749786 0.499857 0.499998
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O 0.749786 0.249929 0.545440
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O 0.749786 0.000000 0.590882
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O 0.749786 0.499857 0.590882
O 0.000000 0.249929 0.590882
O 0.000000 0.749786 0.590882
O 0.499857 0.749786 0.590882
O 0.499857 0.249929 0.590882
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O 0.250185 0.251244 0.636319
O 0.251997 0.751670 0.636548
O 0.750331 0.752258 0.636548
O 0.502637 0.252640 0.681120
O 0.752526 0.503144 0.681374
O 0.253823 0.503290 0.681624
O 0.252500 0.003221 0.681898
O 0.002897 0.752762 0.682063
O 0.003026 0.254072 0.682107
O 0.753775 0.003295 0.682140
O 0.502919 0.754233 0.682595
O 0.255756 0.256256 0.726840

O 0.748514 0.257802 0.726840
O 0.250238 0.751591 0.728234
O 0.753664 0.749734 0.728269
O 0.750223 0.007729 0.770019
O 0.254742 0.007403 0.770237
O 0.005115 0.252659 0.771130
O 0.245944 0.507577 0.771549
O 0.760503 0.506802 0.771903
O 0.501966 0.754518 0.772150
O 0.505027 0.260165 0.772460
O 0.001533 0.763311 0.774875
O 0.355308 0.759845 0.815740
O 0.647693 0.759734 0.815808

Structure 21. TiO_2-terminated $SrTiO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   7.89043600
_cell_length_b   7.89043600
_cell_length_c   43.39739600
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.499472  0.496750  0.272174
  Sr  0.999482  0.996759  0.272175
  Sr  0.999539  0.486868  0.273260
  Sr  0.499526  0.986870  0.273260
  Sr  0.499193  0.497177  0.363568
  Sr  0.999206  0.997188  0.363603
  Sr  0.999193  0.496546  0.363698
  Sr  0.499177  0.996568  0.363698
  Sr  0.000000  0.499857  0.454560
  Sr  0.000000  0.000000  0.454560
  Sr  0.499857  0.000000  0.454560
  Sr  0.499857  0.499857  0.454560
  Sr  0.000000  0.000000  0.545440
  Sr  0.000000  0.499857  0.545440
  Sr  0.499857  0.000000  0.545440
  Sr  0.499857  0.499857  0.545440
  Sr  0.499177  0.996568  0.636302
  Sr  0.999193  0.496546  0.636302
  Sr  0.999206  0.997188  0.636397
  Sr  0.499193  0.497177  0.636432
  Sr  0.499526  0.986870  0.726740
  Sr  0.999539  0.486868  0.726740
  Sr  0.999482  0.996759  0.727825
  Sr  0.499472  0.496750  0.727826
  Ti  0.771271  0.733977  0.227639
  Ti  0.271307  0.233972  0.227645
  Ti  0.728519  0.233989  0.227649
  Ti  0.228509  0.733981  0.227652
  Ti  0.749494  0.742435  0.318076
  Ti  0.249477  0.242426  0.318083
  Ti  0.747527  0.242405  0.318087
  Ti  0.247523  0.742418  0.318087
  Ti  0.249929  0.749786  0.409119
```

Ti 0.249929 0.249929 0.409119
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Ti 0.749786 0.749786 0.409119
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Ti 0.249929 0.749786 0.499998
Ti 0.749786 0.749786 0.499998
Ti 0.749786 0.249929 0.499998
Ti 0.249929 0.249929 0.590881
Ti 0.249929 0.749786 0.590881
Ti 0.749786 0.249929 0.590881
Ti 0.749786 0.749786 0.590881
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Ti 0.747527 0.242405 0.681913
Ti 0.249477 0.242426 0.681917
Ti 0.749494 0.742435 0.681924
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Ti 0.728519 0.233989 0.772351
Ti 0.271307 0.233972 0.772355
Ti 0.771271 0.733977 0.772361
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C 0.999909 0.249710 0.197738
C 0.999909 0.249710 0.802262
C 0.499907 0.749667 0.802268
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O 0.145990 0.252651 0.185585
O 0.353822 0.752553 0.185586
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O 0.499908 0.281952 0.225314
O 0.999906 0.781930 0.225322
O 0.499918 0.740873 0.229225
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O 0.229077 0.509067 0.230378
O 0.729073 0.009053 0.230380
O 0.245246 0.755678 0.272509
O 0.745229 0.255682 0.272510
O 0.254995 0.255617 0.272512
O 0.754963 0.755607 0.272517
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O 0.500421 0.756470 0.317458
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O 0.000000 0.249929 0.590881
O 0.499857 0.749786 0.590881
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O 0.751509 0.251688 0.636421
O 0.248844 0.251727 0.636433
O 0.000328 0.749709 0.681369
O 0.500345 0.249707 0.681375
O 0.746633 0.503381 0.681704
O 0.246631 0.003365 0.681707
O 0.754024 0.003403 0.681719

O 0.254022 0.503416 0.681726
O 0.500421 0.756470 0.682542
O 0.000409 0.256472 0.682547
O 0.754963 0.755607 0.727483
O 0.254995 0.255617 0.727488
O 0.745229 0.255682 0.727490
O 0.245246 0.755678 0.727491
O 0.729073 0.009053 0.769620
O 0.229077 0.509067 0.769622
O 0.770705 0.509068 0.769642
O 0.270712 0.009066 0.769644
O 0.999920 0.240885 0.770769
O 0.499918 0.740873 0.770775
O 0.999906 0.781930 0.774678
O 0.499908 0.281952 0.774686
O 0.853816 0.252606 0.814409
O 0.353822 0.752553 0.814414
O 0.145990 0.252651 0.814415
O 0.645980 0.752595 0.814418

Structure 22. ZrO_2-terminated $SrZrO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.39465800
_cell_length_b   8.39465800
_cell_length_c   46.17061600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.000000  0.000000  0.545455
  Sr  0.996835  0.003177  0.637213
  Sr  0.999904  0.998202  0.729607
  Sr  0.000000  0.500000  0.545455
  Sr  0.998572  0.478496  0.636594
  Sr  0.000568  0.494508  0.730883
  Sr  0.500000  0.000000  0.545455
  Sr  0.499258  0.985873  0.634994
  Sr  0.500883  0.000840  0.729546
  Sr  0.500000  0.500000  0.545455
  Sr  0.496580  0.509113  0.636671
  Sr  0.498849  0.508141  0.727159
  Sr  0.000000  0.000000  0.454545
  Sr  0.996835  0.003177  0.362787
  Sr  0.999904  0.998202  0.270393
  Sr  0.000000  0.500000  0.454545
  Sr  0.998572  0.478496  0.363406
  Sr  0.000568  0.494508  0.269117
  Sr  0.500000  0.000000  0.454545
  Sr  0.499258  0.985873  0.365006
  Sr  0.500883  0.000840  0.270454
  Sr  0.500000  0.500000  0.454545
  Sr  0.496580  0.509113  0.363329
  Sr  0.498849  0.508141  0.272841
  Zr  0.250000  0.250000  0.500000
  Zr  0.250000  0.250000  0.590909
  Zr  0.252478  0.248342  0.681117
  Zr  0.259130  0.248813  0.768838
  Zr  0.250000  0.750000  0.500000
  Zr  0.250000  0.750000  0.590909
  Zr  0.245925  0.749325  0.680877
  Zr  0.243454  0.748269  0.768587
  Zr  0.750000  0.250000  0.500000
```

Zr 0.750000 0.250000 0.590909
Zr 0.746070 0.248561 0.681122
Zr 0.741419 0.249971 0.768928
Zr 0.750000 0.750000 0.500000
Zr 0.750000 0.750000 0.590909
Zr 0.752308 0.748950 0.680910
Zr 0.756132 0.746982 0.768632
Zr 0.250000 0.250000 0.409091
Zr 0.252478 0.248342 0.318883
Zr 0.259130 0.248813 0.231162
Zr 0.250000 0.750000 0.409091
Zr 0.245925 0.749325 0.319123
Zr 0.243454 0.748269 0.231413
Zr 0.750000 0.250000 0.409091
Zr 0.746070 0.248561 0.318878
Zr 0.741419 0.249971 0.231072
Zr 0.750000 0.750000 0.409091
Zr 0.752308 0.748950 0.319090
Zr 0.756132 0.746982 0.231368
O 0.250000 0.000000 0.500000
O 0.250000 0.000000 0.590909
O 0.202209 0.000346 0.682164
O 0.252710 0.997875 0.765913
O 0.250000 0.500000 0.500000
O 0.250000 0.500000 0.590909
O 0.297416 0.500441 0.680661
O 0.248105 0.497897 0.768158
O 0.750000 0.000000 0.500000
O 0.750000 0.000000 0.590909
O 0.796605 0.000344 0.683678
O 0.748276 0.997935 0.764966
O 0.750000 0.500000 0.500000
O 0.750000 0.500000 0.590909
O 0.702410 0.500239 0.679044
O 0.753647 0.497818 0.769983
O 0.250000 0.250000 0.545455
O 0.220512 0.253328 0.636625
O 0.302226 0.253479 0.726370
O 0.250000 0.750000 0.545455
O 0.283816 0.757499 0.636557
O 0.200066 0.739851 0.726176
O 0.750000 0.250000 0.545455
O 0.782175 0.246139 0.636667
O 0.698788 0.262058 0.726468
O 0.750000 0.750000 0.545455
O 0.718946 0.764895 0.636563

O 0.797721 0.731188 0.726228
O 0.000000 0.250000 0.500000
O 0.000000 0.250000 0.590909
O 0.000052 0.295188 0.687341
O 0.000520 0.245133 0.764503
O 0.000000 0.750000 0.500000
O 0.000000 0.750000 0.590909
O 0.999711 0.708946 0.672833
O 0.000126 0.754592 0.777342
O 0.500000 0.250000 0.500000
O 0.500000 0.250000 0.590909
O 0.500060 0.202343 0.674136
O 0.500330 0.243518 0.778914
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
O 0.499877 0.788832 0.688350
O 0.500104 0.747509 0.764011
O 0.250000 0.000000 0.409091
O 0.202209 0.000346 0.317836
O 0.252710 0.997875 0.234087
O 0.250000 0.500000 0.409091
O 0.297416 0.500441 0.319339
O 0.248105 0.497897 0.231842
O 0.750000 0.000000 0.409091
O 0.796605 0.000344 0.316322
O 0.748276 0.997935 0.235034
O 0.750000 0.500000 0.409091
O 0.702410 0.500239 0.320956
O 0.753647 0.497818 0.230017
O 0.250000 0.250000 0.454545
O 0.220512 0.253328 0.363375
O 0.302226 0.253479 0.273630
O 0.250000 0.750000 0.454545
O 0.283816 0.757499 0.363443
O 0.200066 0.739851 0.273824
O 0.750000 0.250000 0.454545
O 0.782175 0.246139 0.363333
O 0.698788 0.262058 0.273532
O 0.750000 0.750000 0.454545
O 0.718946 0.764895 0.363437
O 0.797721 0.731188 0.273772
O 0.000000 0.250000 0.409091
O 0.000052 0.295188 0.312659
O 0.000520 0.245133 0.235497
O 0.000000 0.750000 0.409091
O 0.999711 0.708946 0.327167

O 0.000126 0.754592 0.222658
O 0.500000 0.250000 0.409091
O 0.500060 0.202343 0.325864
O 0.500330 0.243518 0.221086
O 0.500000 0.750000 0.409091
O 0.499877 0.788832 0.311650
O 0.500104 0.747509 0.235989

Structure 23. ZrO_2-terminated $SrZrO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.39465800
_cell_length_b   8.39465800
_cell_length_c   46.17061600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.500013  0.997772  0.269879
  Sr  0.999923  0.491935  0.273026
  Sr  0.500149  0.503863  0.271053
  Sr  0.000171  0.004715  0.274042
  Sr  0.500562  0.497294  0.363317
  Sr  0.000562  0.989169  0.363249
  Sr  0.500106  0.016207  0.364393
  Sr  0.000148  0.519149  0.363962
  Sr  0.500000  0.500000  0.454545
  Sr  0.500000  0.000000  0.454545
  Sr  0.000000  0.500000  0.454545
  Sr  0.000000  0.000000  0.454545
  Sr  0.500000  0.500000  0.545455
  Sr  0.500000  0.000000  0.545455
  Sr  0.000000  0.500000  0.545455
  Sr  0.000000  0.000000  0.545455
  Sr  0.000148  0.519149  0.636038
  Sr  0.500106  0.016207  0.635607
  Sr  0.000562  0.989169  0.636751
  Sr  0.500562  0.497294  0.636683
  Sr  0.000171  0.004715  0.725958
  Sr  0.500149  0.503863  0.728947
  Sr  0.999923  0.491935  0.726974
  Sr  0.500013  0.997772  0.730121
  Zr  0.235843  0.751092  0.230321
  Zr  0.764292  0.751207  0.230319
  Zr  0.757671  0.250457  0.231380
  Zr  0.242445  0.250563  0.231386
  Zr  0.249447  0.251011  0.319229
  Zr  0.750896  0.250999  0.319232
  Zr  0.746086  0.751400  0.318394
  Zr  0.254266  0.751354  0.318396
  Zr  0.250000  0.250000  0.409091
```

Zr 0.250000 0.750000 0.409091
Zr 0.750000 0.250000 0.409091
Zr 0.750000 0.750000 0.409091
Zr 0.250000 0.250000 0.500000
Zr 0.250000 0.750000 0.500000
Zr 0.750000 0.250000 0.500000
Zr 0.750000 0.750000 0.500000
Zr 0.250000 0.250000 0.590909
Zr 0.250000 0.750000 0.590909
Zr 0.750000 0.250000 0.590909
Zr 0.750000 0.750000 0.590909
Zr 0.254266 0.751354 0.681604
Zr 0.746086 0.751400 0.681606
Zr 0.750896 0.250999 0.680768
Zr 0.249447 0.251011 0.680771
Zr 0.242445 0.250563 0.768614
Zr 0.757671 0.250457 0.768620
Zr 0.764292 0.751207 0.769681
Zr 0.235843 0.751092 0.769679
C 0.500075 0.743314 0.197621
C 0.500075 0.743314 0.802379
O 0.637894 0.745813 0.186131
O 0.362256 0.746182 0.186132
O 0.500071 0.738954 0.227151
O 0.000039 0.245381 0.222599
O 0.744536 0.999515 0.232998
O 0.255388 0.999494 0.233154
O 0.241583 0.502151 0.234086
O 0.758428 0.502165 0.234217
O 0.000062 0.756799 0.238822
O 0.500027 0.256299 0.235570
O 0.297749 0.754010 0.273354
O 0.799579 0.248253 0.273936
O 0.702530 0.754950 0.273354
O 0.200568 0.249088 0.273943
O 0.000098 0.705962 0.313122
O 0.500084 0.203314 0.312641
O 0.701170 0.499286 0.318076
O 0.199710 0.999724 0.318981
O 0.299141 0.499288 0.318289
O 0.800611 0.999757 0.319173
O 0.000075 0.299236 0.325210
O 0.500109 0.797009 0.325797
O 0.221906 0.743969 0.363358
O 0.718676 0.246379 0.363473
O 0.777741 0.742773 0.363358

O 0.280893 0.245162 0.363477
O 0.250000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.250000 0.500000 0.409091
O 0.750000 0.000000 0.409091
O 0.500000 0.250000 0.409091
O 0.500000 0.750000 0.409091
O 0.000000 0.750000 0.409091
O 0.000000 0.250000 0.409091
O 0.750000 0.250000 0.454545
O 0.750000 0.750000 0.454545
O 0.250000 0.750000 0.454545
O 0.250000 0.250000 0.454545
O 0.250000 0.500000 0.500000
O 0.250000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.500000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.000000 0.250000 0.500000
O 0.000000 0.750000 0.500000
O 0.250000 0.250000 0.545455
O 0.250000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.750000 0.750000 0.545455
O 0.250000 0.500000 0.590909
O 0.250000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.750000 0.000000 0.590909
O 0.500000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.000000 0.250000 0.590909
O 0.000000 0.750000 0.590909
O 0.280893 0.245162 0.636523
O 0.777741 0.742773 0.636642
O 0.718676 0.246379 0.636527
O 0.221906 0.743969 0.636642
O 0.500109 0.797009 0.674203
O 0.000075 0.299236 0.674790
O 0.800611 0.999757 0.680827
O 0.299141 0.499288 0.681711
O 0.199710 0.999724 0.681019
O 0.701170 0.499286 0.681924
O 0.500084 0.203314 0.687359
O 0.000098 0.705962 0.686878
O 0.200568 0.249088 0.726057

O 0.702530 0.754950 0.726646
O 0.799579 0.248253 0.726064
O 0.297749 0.754010 0.726646
O 0.500027 0.256299 0.764430
O 0.000062 0.756799 0.761178
O 0.758428 0.502165 0.765783
O 0.241583 0.502151 0.765914
O 0.255388 0.999494 0.766846
O 0.744536 0.999515 0.767002
O 0.000039 0.245381 0.777401
O 0.500071 0.738954 0.772849
O 0.362256 0.746182 0.813868
O 0.637894 0.745813 0.813869

Structure 24. ZrO_2-terminated $SrZrO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.39465800
_cell_length_b   8.39465800
_cell_length_c   46.17061600
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.999773  0.489837  0.272729
  Sr  0.499822  0.988843  0.272822
  Sr  0.000588  0.012225  0.273430
  Sr  0.500650  0.510800  0.273694
  Sr  0.002493  0.995304  0.363493
  Sr  0.502450  0.493797  0.363604
  Sr  0.000419  0.518320  0.364009
  Sr  0.500316  0.016712  0.364319
  Sr  0.000000  0.000000  0.454545
  Sr  0.000000  0.500000  0.454545
  Sr  0.500000  0.000000  0.454545
  Sr  0.500000  0.500000  0.454545
  Sr  0.000000  0.000000  0.545455
  Sr  0.000000  0.500000  0.545455
  Sr  0.500000  0.000000  0.545455
  Sr  0.500000  0.500000  0.545455
  Sr  0.500316  0.016712  0.635681
  Sr  0.000419  0.518320  0.635991
  Sr  0.502450  0.493797  0.636396
  Sr  0.002493  0.995304  0.636507
  Sr  0.500650  0.510800  0.726306
  Sr  0.000588  0.012225  0.726570
  Sr  0.499822  0.988843  0.727178
  Sr  0.999773  0.489837  0.727271
  Zr  0.736470  0.251980  0.230478
  Zr  0.263705  0.252305  0.230488
  Zr  0.236462  0.751803  0.230489
  Zr  0.763694  0.752082  0.230491
  Zr  0.749089  0.751899  0.318700
  Zr  0.252085  0.751736  0.318705
  Zr  0.249145  0.251716  0.318706
  Zr  0.751986  0.251529  0.318713
  Zr  0.750000  0.750000  0.409091
```

Zr 0.750000 0.250000 0.409091
Zr 0.250000 0.750000 0.409091
Zr 0.250000 0.250000 0.409091
Zr 0.750000 0.750000 0.500000
Zr 0.750000 0.250000 0.500000
Zr 0.250000 0.750000 0.500000
Zr 0.250000 0.250000 0.500000
Zr 0.750000 0.750000 0.590909
Zr 0.750000 0.250000 0.590909
Zr 0.250000 0.750000 0.590909
Zr 0.250000 0.250000 0.590909
Zr 0.751986 0.251529 0.681287
Zr 0.249145 0.251716 0.681294
Zr 0.252085 0.751736 0.681295
Zr 0.749089 0.751899 0.681300
Zr 0.763694 0.752082 0.769509
Zr 0.236462 0.751803 0.769511
Zr 0.263705 0.252305 0.769512
Zr 0.736470 0.251980 0.769522
C 0.000131 0.241767 0.198208
C 0.500109 0.743552 0.198219
C 0.500109 0.743552 0.801781
C 0.000131 0.241767 0.801792
O 0.137926 0.247146 0.186834
O 0.862344 0.247937 0.186837
O 0.637890 0.749119 0.186841
O 0.362312 0.749922 0.186852
O 0.000081 0.231231 0.227786
O 0.500076 0.732322 0.227788
O 0.237166 0.500739 0.233806
O 0.762444 0.500717 0.234133
O 0.737588 0.000729 0.234224
O 0.262060 0.000758 0.234546
O 0.500069 0.262322 0.238290
O 0.000060 0.762447 0.238333
O 0.796835 0.251411 0.273643
O 0.296707 0.748781 0.273651
O 0.203578 0.253523 0.273660
O 0.703700 0.750781 0.273661
O 0.500234 0.203324 0.313268
O 0.000273 0.702241 0.313568
O 0.199404 0.999758 0.318241
O 0.699482 0.499756 0.318695
O 0.801709 0.999821 0.318810
O 0.301571 0.499825 0.319297
O 0.500279 0.800799 0.324620

O 0.000242 0.299785 0.324850
O 0.721479 0.245343 0.363435
O 0.222169 0.747609 0.363441
O 0.276784 0.241061 0.363441
O 0.776353 0.743392 0.363445
O 0.750000 0.500000 0.409091
O 0.250000 0.000000 0.409091
O 0.750000 0.000000 0.409091
O 0.250000 0.500000 0.409091
O 0.000000 0.750000 0.409091
O 0.000000 0.250000 0.409091
O 0.500000 0.250000 0.409091
O 0.500000 0.750000 0.409091
O 0.250000 0.750000 0.454545
O 0.250000 0.250000 0.454545
O 0.750000 0.250000 0.454545
O 0.750000 0.750000 0.454545
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.250000 0.000000 0.500000
O 0.250000 0.500000 0.500000
O 0.000000 0.750000 0.500000
O 0.000000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.750000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.250000 0.750000 0.545455
O 0.250000 0.250000 0.545455
O 0.750000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.250000 0.000000 0.590909
O 0.250000 0.500000 0.590909
O 0.000000 0.750000 0.590909
O 0.000000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.500000 0.250000 0.590909
O 0.776353 0.743392 0.636555
O 0.276784 0.241061 0.636559
O 0.222169 0.747609 0.636559
O 0.721479 0.245343 0.636565
O 0.000242 0.299785 0.675150
O 0.500279 0.800799 0.675380
O 0.301571 0.499825 0.680703
O 0.801709 0.999821 0.681190
O 0.699482 0.499756 0.681305

O 0.199404 0.999758 0.681759
O 0.000273 0.702241 0.686432
O 0.500234 0.203324 0.686732
O 0.703700 0.750781 0.726339
O 0.203578 0.253523 0.726340
O 0.296707 0.748781 0.726349
O 0.796835 0.251411 0.726357
O 0.000060 0.762447 0.761667
O 0.500069 0.262322 0.761710
O 0.262060 0.000758 0.765454
O 0.737588 0.000729 0.765776
O 0.762444 0.500717 0.765867
O 0.237166 0.500739 0.766194
O 0.500076 0.732322 0.772212
O 0.000081 0.231231 0.772214
O 0.362312 0.749922 0.813148
O 0.637890 0.749119 0.813159
O 0.862344 0.247937 0.813163
O 0.137926 0.247146 0.813166

Structure 25. HfO_2-terminated $SrHfO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.500000  0.500000  0.545455
  Sr  0.498902  0.503017  0.636558
  Sr  0.498566  0.503783  0.728855
  Sr  0.500000  0.000000  0.545455
  Sr  0.499398  0.988516  0.635898
  Sr  0.498690  0.001926  0.729953
  Sr  0.000000  0.500000  0.545455
  Sr  0.999430  0.486833  0.636292
  Sr  0.998581  0.499448  0.730273
  Sr  0.000000  0.000000  0.545455
  Sr  0.998940  0.001655  0.636742
  Sr  0.998548  0.000332  0.729618
  Sr  0.500000  0.500000  0.454545
  Sr  0.498902  0.503017  0.363442
  Sr  0.498566  0.503783  0.271145
  Sr  0.500000  0.000000  0.454545
  Sr  0.499398  0.988516  0.364102
  Sr  0.498690  0.001926  0.270047
  Sr  0.000000  0.500000  0.454545
  Sr  0.999430  0.486833  0.363708
  Sr  0.998581  0.499448  0.269727
  Sr  0.000000  0.000000  0.454545
  Sr  0.998940  0.001655  0.363258
  Sr  0.998548  0.000332  0.270382
  Hf  0.250000  0.250000  0.500000
  Hf  0.250000  0.750000  0.500000
  Hf  0.750000  0.250000  0.500000
  Hf  0.750000  0.750000  0.500000
  Hf  0.750000  0.750000  0.590909
  Hf  0.750948  0.749333  0.681176
  Hf  0.753465  0.749326  0.769321
  Hf  0.750000  0.250000  0.590909
  Hf  0.746788  0.249323  0.681224
```

Hf 0.742885 0.250422 0.769378
Hf 0.250000 0.750000 0.590909
Hf 0.246780 0.749413 0.681167
Hf 0.243493 0.749485 0.769298
Hf 0.250000 0.250000 0.590909
Hf 0.251009 0.249224 0.681216
Hf 0.254159 0.250263 0.769356
Hf 0.750000 0.750000 0.409091
Hf 0.750948 0.749333 0.318824
Hf 0.753465 0.749326 0.230679
Hf 0.750000 0.250000 0.409091
Hf 0.746788 0.249323 0.318776
Hf 0.742885 0.250422 0.230622
Hf 0.250000 0.750000 0.409091
Hf 0.246780 0.749413 0.318833
Hf 0.243493 0.749485 0.230702
Hf 0.250000 0.250000 0.409091
Hf 0.251009 0.249224 0.318784
Hf 0.254159 0.250263 0.230644
O 0.250000 0.000000 0.500000
O 0.250000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.000000 0.250000 0.500000
O 0.000000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
O 0.498857 0.790068 0.686572
O 0.498481 0.748592 0.766040
O 0.500000 0.250000 0.590909
O 0.498968 0.206110 0.676332
O 0.498506 0.249641 0.776771
O 0.000000 0.750000 0.590909
O 0.998901 0.707901 0.675973
O 0.998497 0.753065 0.776386
O 0.000000 0.250000 0.590909
O 0.998905 0.291550 0.686281
O 0.998527 0.247771 0.766120
O 0.750000 0.750000 0.545455
O 0.728232 0.756774 0.636499
O 0.785254 0.743174 0.726697
O 0.750000 0.250000 0.545455
O 0.770597 0.251625 0.636527
O 0.711087 0.253544 0.726738
O 0.250000 0.750000 0.545455

O 0.270852 0.755792 0.636500
O 0.211731 0.744368 0.726672
O 0.250000 0.250000 0.545455
O 0.228540 0.252477 0.636510
O 0.286287 0.252358 0.726722
O 0.750000 0.500000 0.590909
O 0.704766 0.500319 0.680849
O 0.750602 0.499604 0.769804
O 0.750000 0.000000 0.590909
O 0.792540 0.000326 0.682248
O 0.746574 0.999573 0.768206
O 0.250000 0.500000 0.590909
O 0.292817 0.500316 0.680998
O 0.246425 0.499593 0.769562
O 0.250000 0.000000 0.590909
O 0.204966 0.000322 0.682023
O 0.250459 0.999579 0.768321
O 0.500000 0.750000 0.409091
O 0.498857 0.790068 0.313428
O 0.498481 0.748592 0.233960
O 0.500000 0.250000 0.409091
O 0.498968 0.206110 0.323668
O 0.498506 0.249641 0.223229
O 0.000000 0.750000 0.409091
O 0.998901 0.707901 0.324027
O 0.998497 0.753065 0.223614
O 0.000000 0.250000 0.409091
O 0.998905 0.291550 0.313719
O 0.998527 0.247771 0.233880
O 0.750000 0.750000 0.454545
O 0.728232 0.756774 0.363501
O 0.785254 0.743174 0.273303
O 0.750000 0.250000 0.454545
O 0.770597 0.251625 0.363473
O 0.711087 0.253544 0.273262
O 0.250000 0.750000 0.454545
O 0.270852 0.755792 0.363500
O 0.211731 0.744368 0.273328
O 0.250000 0.250000 0.454545
O 0.228540 0.252477 0.363490
O 0.286287 0.252358 0.273278
O 0.750000 0.500000 0.409091
O 0.704766 0.500319 0.319151
O 0.750602 0.499604 0.230196
O 0.750000 0.000000 0.409091
O 0.792540 0.000326 0.317752

O 0.746574 0.999573 0.231794
O 0.250000 0.500000 0.409091
O 0.292817 0.500316 0.319002
O 0.246425 0.499593 0.230438
O 0.250000 0.000000 0.409091
O 0.204966 0.000322 0.317977
O 0.250459 0.999579 0.231679

Structure 26. HfO_2-terminated $SrHfO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.500000  0.500000  0.545455
  Sr  0.499269  0.500105  0.636391
  Sr  0.499089  0.499834  0.728847
  Sr  0.500000  0.000000  0.545455
  Sr  0.499644  0.009411  0.635711
  Sr  0.499138  0.996016  0.729532
  Sr  0.000000  0.500000  0.545455
  Sr  0.999633  0.514356  0.636384
  Sr  0.999162  0.492535  0.727926
  Sr  0.000000  0.000000  0.545455
  Sr  0.999282  0.995506  0.636554
  Sr  0.999090  0.005949  0.727588
  Sr  0.500000  0.500000  0.454545
  Sr  0.499269  0.500105  0.363609
  Sr  0.499089  0.499834  0.271153
  Sr  0.500000  0.000000  0.454545
  Sr  0.499644  0.009411  0.364289
  Sr  0.499138  0.996016  0.270468
  Sr  0.000000  0.500000  0.454545
  Sr  0.999633  0.514356  0.363616
  Sr  0.999162  0.492535  0.272074
  Sr  0.000000  0.000000  0.454545
  Sr  0.999282  0.995506  0.363446
  Sr  0.999090  0.005949  0.272412
  Hf  0.250000  0.750000  0.500000
  Hf  0.250000  0.250000  0.500000
  Hf  0.750000  0.750000  0.500000
  Hf  0.750000  0.250000  0.500000
  Hf  0.750000  0.250000  0.590909
  Hf  0.749909  0.250625  0.680932
  Hf  0.753995  0.250090  0.769112
  Hf  0.750000  0.750000  0.590909
  Hf  0.746461  0.751028  0.681885
```

Hf 0.762433 0.749917 0.770625
Hf 0.250000 0.250000 0.590909
Hf 0.248655 0.250588 0.680932
Hf 0.244056 0.250014 0.769111
Hf 0.250000 0.750000 0.590909
Hf 0.252123 0.751080 0.681885
Hf 0.235606 0.749974 0.770620
Hf 0.750000 0.250000 0.409091
Hf 0.749909 0.250625 0.319068
Hf 0.753995 0.250090 0.230888
Hf 0.750000 0.750000 0.409091
Hf 0.746461 0.751028 0.318114
Hf 0.762433 0.749917 0.229375
Hf 0.250000 0.250000 0.409091
Hf 0.248655 0.250588 0.319068
Hf 0.244056 0.250014 0.230889
Hf 0.250000 0.750000 0.409091
Hf 0.252123 0.751080 0.318115
Hf 0.235606 0.749974 0.229380
C 0.498961 0.749908 0.803368
C 0.498961 0.749908 0.196632
O 0.498999 0.747126 0.773328
O 0.638719 0.751367 0.814875
O 0.359163 0.751108 0.814863
O 0.498999 0.747126 0.226672
O 0.638719 0.751367 0.185125
O 0.359163 0.751108 0.185137
O 0.250000 0.000000 0.500000
O 0.250000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.000000 0.750000 0.500000
O 0.000000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.500000 0.250000 0.590909
O 0.499285 0.208373 0.686261
O 0.499015 0.252297 0.766070
O 0.500000 0.750000 0.590909
O 0.499332 0.795304 0.676756
O 0.000000 0.250000 0.590909
O 0.999314 0.294830 0.676738
O 0.999010 0.246615 0.775638
O 0.000000 0.750000 0.590909
O 0.999300 0.708646 0.686124
O 0.999014 0.753220 0.764242

O 0.750000 0.250000 0.545455
O 0.729223 0.244204 0.636411
O 0.785150 0.253149 0.726378
O 0.750000 0.750000 0.545455
O 0.768379 0.747610 0.636648
O 0.711204 0.749182 0.727200
O 0.250000 0.250000 0.545455
O 0.270244 0.244907 0.636416
O 0.213035 0.252600 0.726375
O 0.250000 0.750000 0.545455
O 0.231060 0.747033 0.636643
O 0.287077 0.749716 0.727201
O 0.750000 0.500000 0.590909
O 0.704972 0.499764 0.681134
O 0.752848 0.501118 0.768258
O 0.750000 0.000000 0.590909
O 0.794528 0.000072 0.681783
O 0.747057 0.999268 0.767677
O 0.250000 0.500000 0.590909
O 0.293503 0.499767 0.681243
O 0.245089 0.501121 0.768167
O 0.250000 0.000000 0.590909
O 0.203963 0.000080 0.681673
O 0.251002 0.999274 0.767749
O 0.500000 0.250000 0.409091
O 0.499285 0.208373 0.313739
O 0.499015 0.252297 0.233930
O 0.500000 0.750000 0.409091
O 0.499332 0.795304 0.323244
O 0.000000 0.250000 0.409091
O 0.999314 0.294830 0.323262
O 0.999010 0.246615 0.224362
O 0.000000 0.750000 0.409091
O 0.999300 0.708646 0.313876
O 0.999014 0.753220 0.235758
O 0.750000 0.250000 0.454545
O 0.729223 0.244204 0.363589
O 0.785150 0.253149 0.273622
O 0.750000 0.750000 0.454545
O 0.768379 0.747610 0.363352
O 0.711204 0.749182 0.272800
O 0.250000 0.250000 0.454545
O 0.270244 0.244907 0.363584
O 0.213035 0.252600 0.273625
O 0.250000 0.750000 0.454545
O 0.231060 0.747033 0.363357

O 0.287077 0.749716 0.272799
O 0.750000 0.500000 0.409091
O 0.704972 0.499764 0.318866
O 0.752848 0.501118 0.231742
O 0.750000 0.000000 0.409091
O 0.794528 0.000072 0.318217
O 0.747057 0.999268 0.232323
O 0.250000 0.500000 0.409091
O 0.293503 0.499767 0.318757
O 0.245089 0.501121 0.231833
O 0.250000 0.000000 0.409091
O 0.203963 0.000080 0.318327
O 0.251002 0.999274 0.232251

Structure 27. HfO_2-terminated $SrHfO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.28657000
_cell_length_b   8.28657000
_cell_length_c   45.57613800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Sr  0.000309  0.490353  0.272457
  Sr  0.500298  0.990045  0.272489
  Sr  0.000403  0.007825  0.272998
  Sr  0.500411  0.507342  0.273089
  Sr  0.000446  0.998174  0.363762
  Sr  0.500448  0.497675  0.363785
  Sr  0.000166  0.511858  0.364045
  Sr  0.500177  0.011274  0.364168
  Sr  0.500000  0.500000  0.454545
  Sr  0.500000  0.000000  0.454545
  Sr  0.000000  0.500000  0.454545
  Sr  0.000000  0.000000  0.454545
  Sr  0.500000  0.500000  0.545455
  Sr  0.500000  0.000000  0.545455
  Sr  0.000000  0.500000  0.545455
  Sr  0.000000  0.000000  0.545455
  Sr  0.500177  0.011274  0.635832
  Sr  0.000166  0.511858  0.635955
  Sr  0.500448  0.497675  0.636215
  Sr  0.000446  0.998174  0.636238
  Sr  0.500411  0.507342  0.726911
  Sr  0.000403  0.007825  0.727002
  Sr  0.500298  0.990045  0.727511
  Sr  0.000309  0.490353  0.727543
  Hf  0.263563  0.250464  0.229769
  Hf  0.237174  0.750312  0.229770
  Hf  0.763548  0.750361  0.229770
  Hf  0.737153  0.250426  0.229770
  Hf  0.251716  0.750858  0.318520
  Hf  0.749029  0.750903  0.318520
  Hf  0.249038  0.250811  0.318522
  Hf  0.751710  0.250776  0.318523
  Hf  0.250000  0.250000  0.409091
```

Hf 0.250000 0.750000 0.409091
Hf 0.750000 0.250000 0.409091
Hf 0.750000 0.750000 0.409091
Hf 0.750000 0.750000 0.500000
Hf 0.750000 0.250000 0.500000
Hf 0.250000 0.750000 0.500000
Hf 0.250000 0.250000 0.500000
Hf 0.250000 0.250000 0.590909
Hf 0.250000 0.750000 0.590909
Hf 0.750000 0.250000 0.590909
Hf 0.750000 0.750000 0.590909
Hf 0.751710 0.250776 0.681477
Hf 0.249038 0.250811 0.681478
Hf 0.749029 0.750903 0.681480
Hf 0.251716 0.750858 0.681480
Hf 0.737153 0.250426 0.770230
Hf 0.763548 0.750361 0.770230
Hf 0.237174 0.750312 0.770230
Hf 0.263563 0.250464 0.770231
C 0.000350 0.245357 0.197380
C 0.500362 0.745615 0.197381
C 0.500362 0.745615 0.802619
C 0.000350 0.245357 0.802620
O 0.140152 0.248586 0.186005
O 0.640150 0.748848 0.186005
O 0.860557 0.248651 0.186005
O 0.360578 0.748904 0.186006
O 0.500361 0.739480 0.227547
O 0.000355 0.239268 0.227548
O 0.242155 0.500237 0.232837
O 0.758533 0.500245 0.232874
O 0.742230 0.000248 0.232968
O 0.258464 0.000245 0.233004
O 0.000361 0.758519 0.235853
O 0.500358 0.258476 0.235855
O 0.788262 0.251072 0.273291
O 0.212476 0.251319 0.273291
O 0.288232 0.750056 0.273292
O 0.712510 0.750325 0.273294
O 0.500372 0.208030 0.313968
O 0.000370 0.707598 0.314061
O 0.205063 0.999865 0.318549
O 0.795845 0.999872 0.318621
O 0.705165 0.499876 0.318773
O 0.295742 0.499871 0.318834
O 0.500356 0.795704 0.323101

O 0.000359 0.295467 0.323163
O 0.731049 0.245634 0.363507
O 0.231197 0.746673 0.363508
O 0.269184 0.245184 0.363509
O 0.769041 0.746259 0.363511
O 0.500000 0.750000 0.409091
O 0.000000 0.250000 0.409091
O 0.500000 0.250000 0.409091
O 0.000000 0.750000 0.409091
O 0.250000 0.500000 0.409091
O 0.250000 0.000000 0.409091
O 0.750000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.750000 0.250000 0.454545
O 0.750000 0.750000 0.454545
O 0.250000 0.750000 0.454545
O 0.250000 0.250000 0.454545
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.250000 0.000000 0.500000
O 0.000000 0.750000 0.500000
O 0.250000 0.500000 0.500000
O 0.000000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.250000 0.250000 0.545455
O 0.250000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.750000 0.750000 0.545455
O 0.500000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.000000 0.250000 0.590909
O 0.000000 0.750000 0.590909
O 0.250000 0.500000 0.590909
O 0.250000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.750000 0.000000 0.590909
O 0.769041 0.746259 0.636489
O 0.269184 0.245184 0.636491
O 0.231197 0.746673 0.636492
O 0.731049 0.245634 0.636493
O 0.000359 0.295467 0.676837
O 0.500356 0.795704 0.676899
O 0.295742 0.499871 0.681166
O 0.705165 0.499876 0.681227
O 0.795845 0.999872 0.681379

O 0.205063 0.999865 0.681451
O 0.000370 0.707598 0.685939
O 0.500372 0.208030 0.686032
O 0.712510 0.750325 0.726706
O 0.288232 0.750056 0.726708
O 0.212476 0.251319 0.726709
O 0.788262 0.251072 0.726709
O 0.500358 0.258476 0.764145
O 0.000361 0.758519 0.764147
O 0.258464 0.000245 0.766996
O 0.742230 0.000248 0.767032
O 0.758533 0.500245 0.767126
O 0.242155 0.500237 0.767163
O 0.000355 0.239268 0.772452
O 0.500361 0.739480 0.772453
O 0.360578 0.748904 0.813994
O 0.860557 0.248651 0.813995
O 0.640150 0.748848 0.813995
O 0.140152 0.248586 0.813995

Structure 28. TiO_2-terminated $BaTiO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.07335600
_cell_length_b   8.07335600
_cell_length_c   44.40346100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.000000  0.000000  0.545455
  Ba  0.997165  0.998236  0.636368
  Ba  0.994941  0.001359  0.729666
  Ba  0.000000  0.500000  0.545455
  Ba  0.997167  0.498239  0.636368
  Ba  0.994960  0.501368  0.729662
  Ba  0.500000  0.000000  0.545455
  Ba  0.497175  0.998235  0.636368
  Ba  0.494956  0.001368  0.729669
  Ba  0.500000  0.500000  0.545455
  Ba  0.497165  0.498241  0.636368
  Ba  0.494938  0.501358  0.729665
  Ba  0.000000  0.000000  0.454545
  Ba  0.997165  0.998236  0.363632
  Ba  0.994941  0.001359  0.270334
  Ba  0.000000  0.500000  0.454545
  Ba  0.997167  0.498239  0.363632
  Ba  0.994960  0.501368  0.270338
  Ba  0.500000  0.000000  0.454545
  Ba  0.497175  0.998235  0.363632
  Ba  0.494956  0.001368  0.270331
  Ba  0.500000  0.500000  0.454545
  Ba  0.497165  0.498241  0.363632
  Ba  0.494938  0.501358  0.270335
  Ti  0.250000  0.250000  0.500000
  Ti  0.250000  0.250000  0.590909
  Ti  0.236917  0.239160  0.681460
  Ti  0.236942  0.262199  0.770330
  Ti  0.250000  0.750000  0.500000
  Ti  0.250000  0.750000  0.590909
  Ti  0.236914  0.739173  0.681461
  Ti  0.236951  0.762208  0.770329
  Ti  0.750000  0.250000  0.500000
```

Ti 0.750000 0.250000 0.590909
Ti 0.736911 0.239170 0.681461
Ti 0.736971 0.262223 0.770329
Ti 0.750000 0.750000 0.500000
Ti 0.750000 0.750000 0.590909
Ti 0.736910 0.739166 0.681462
Ti 0.736948 0.762189 0.770329
Ti 0.250000 0.250000 0.409091
Ti 0.236917 0.239160 0.318540
Ti 0.236942 0.262199 0.229670
Ti 0.250000 0.750000 0.409091
Ti 0.236914 0.739173 0.318539
Ti 0.236951 0.762208 0.229671
Ti 0.750000 0.250000 0.409091
Ti 0.736911 0.239170 0.318539
Ti 0.736971 0.262223 0.229671
Ti 0.750000 0.750000 0.409091
Ti 0.736910 0.739166 0.318538
Ti 0.736948 0.762189 0.229672
O 0.250000 0.000000 0.500000
O 0.250000 0.000000 0.590909
O 0.252691 0.009025 0.681804
O 0.255722 0.986999 0.773334
O 0.250000 0.500000 0.500000
O 0.250000 0.500000 0.590909
O 0.252705 0.509035 0.681805
O 0.255739 0.486985 0.773333
O 0.750000 0.000000 0.500000
O 0.750000 0.000000 0.590909
O 0.752704 0.009033 0.681805
O 0.755745 0.986973 0.773332
O 0.750000 0.500000 0.500000
O 0.750000 0.500000 0.590909
O 0.752686 0.509027 0.681803
O 0.755739 0.487013 0.773332
O 0.250000 0.250000 0.545455
O 0.250817 0.251785 0.636291
O 0.251713 0.250809 0.727561
O 0.250000 0.750000 0.545455
O 0.250814 0.751789 0.636291
O 0.251712 0.750822 0.727559
O 0.750000 0.250000 0.545455
O 0.750810 0.251786 0.636291
O 0.751732 0.250828 0.727559
O 0.750000 0.750000 0.545455
O 0.750811 0.751788 0.636291

O 0.751722 0.750806 0.727558
O 0.000000 0.250000 0.500000
O 0.000000 0.250000 0.590909
O 0.007464 0.254363 0.681844
O 0.012342 0.243241 0.773136
O 0.000000 0.750000 0.500000
O 0.000000 0.750000 0.590909
O 0.007456 0.754351 0.681845
O 0.012359 0.743217 0.773135
O 0.500000 0.250000 0.500000
O 0.500000 0.250000 0.590909
O 0.507455 0.254349 0.681846
O 0.512379 0.243234 0.773135
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
O 0.507459 0.754367 0.681846
O 0.512346 0.743233 0.773132
O 0.250000 0.000000 0.409091
O 0.252691 0.009025 0.318196
O 0.255722 0.986999 0.226666
O 0.250000 0.500000 0.409091
O 0.252705 0.509035 0.318195
O 0.255739 0.486985 0.226667
O 0.750000 0.000000 0.409091
O 0.752704 0.009033 0.318195
O 0.755745 0.986973 0.226668
O 0.750000 0.500000 0.409091
O 0.752686 0.509027 0.318197
O 0.755739 0.487013 0.226668
O 0.250000 0.250000 0.454545
O 0.250817 0.251785 0.363709
O 0.251713 0.250809 0.272439
O 0.250000 0.750000 0.454545
O 0.250814 0.751789 0.363709
O 0.251712 0.750822 0.272441
O 0.750000 0.250000 0.454545
O 0.750810 0.251786 0.363709
O 0.751732 0.250828 0.272441
O 0.750000 0.750000 0.454545
O 0.750811 0.751788 0.363709
O 0.751722 0.750806 0.272442
O 0.000000 0.250000 0.409091
O 0.007464 0.254363 0.318156
O 0.012342 0.243241 0.226864
O 0.000000 0.750000 0.409091
O 0.007456 0.754351 0.318155

O 0.012359 0.743217 0.226865
O 0.500000 0.250000 0.409091
O 0.507455 0.254349 0.318154
O 0.512379 0.243234 0.226865
O 0.500000 0.750000 0.409091
O 0.507459 0.754367 0.318154
O 0.512346 0.743233 0.226868

Structure 29. TiO_2-terminated $BaTiO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.07335600
_cell_length_b   8.07335600
_cell_length_c   44.40346100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.497163  0.002704  0.729169
  Ba  0.495664  0.503401  0.728809
  Ba  0.997825  0.007906  0.727807
  Ba  0.995788  0.502658  0.728496
  Ba  0.500000  0.000000  0.545455
  Ba  0.497863  0.000195  0.636286
  Ba  0.500000  0.500000  0.545455
  Ba  0.497864  0.504184  0.636187
  Ba  0.000000  0.000000  0.545455
  Ba  0.997656  0.000438  0.636223
  Ba  0.000000  0.500000  0.545455
  Ba  0.997474  0.503860  0.636212
  Ba  0.497163  0.002704  0.270831
  Ba  0.495664  0.503401  0.271191
  Ba  0.997825  0.007906  0.272193
  Ba  0.995788  0.502658  0.271504
  Ba  0.500000  0.000000  0.454545
  Ba  0.497863  0.000195  0.363714
  Ba  0.500000  0.500000  0.454545
  Ba  0.497864  0.504184  0.363813
  Ba  0.000000  0.000000  0.454545
  Ba  0.997656  0.000438  0.363777
  Ba  0.000000  0.500000  0.454545
  Ba  0.997474  0.503860  0.363788
  Ti  0.771373  0.767132  0.773054
  Ti  0.737204  0.264103  0.769702
  Ti  0.230107  0.766175  0.772882
  Ti  0.235908  0.264215  0.769700
  Ti  0.750000  0.750000  0.500000
  Ti  0.750000  0.750000  0.590909
  Ti  0.738426  0.761620  0.682537
  Ti  0.750000  0.250000  0.500000
  Ti  0.750000  0.250000  0.590909
```

Ti 0.737157 0.261797 0.681015
Ti 0.250000 0.750000 0.500000
Ti 0.250000 0.750000 0.590909
Ti 0.238194 0.761489 0.682361
Ti 0.250000 0.250000 0.500000
Ti 0.250000 0.250000 0.590909
Ti 0.238869 0.262136 0.680941
Ti 0.771373 0.767132 0.226946
Ti 0.737204 0.264103 0.230298
Ti 0.230107 0.766175 0.227118
Ti 0.235908 0.264215 0.230300
Ti 0.750000 0.750000 0.409091
Ti 0.738426 0.761620 0.317463
Ti 0.750000 0.250000 0.409091
Ti 0.737157 0.261797 0.318985
Ti 0.250000 0.750000 0.409091
Ti 0.238194 0.761489 0.317639
Ti 0.250000 0.250000 0.409091
Ti 0.238869 0.262136 0.319059
C 0.500920 0.739174 0.801986
C 0.500920 0.739174 0.198014
O 0.759070 0.987592 0.772517
O 0.753099 0.486061 0.771521
O 0.247239 0.986697 0.772403
O 0.251750 0.486413 0.771554
O 0.754424 0.748247 0.728091
O 0.751028 0.245607 0.726968
O 0.247805 0.747439 0.728123
O 0.253035 0.245806 0.727026
O 0.501544 0.743750 0.771511
O 0.511372 0.241136 0.772699
O 0.000917 0.741893 0.774783
O 0.010568 0.243604 0.772247
O 0.357728 0.738631 0.813904
O 0.644044 0.739571 0.813996
O 0.750000 0.000000 0.500000
O 0.750000 0.000000 0.590909
O 0.752598 0.991945 0.681815
O 0.750000 0.500000 0.500000
O 0.750000 0.500000 0.590909
O 0.752562 0.491931 0.681774
O 0.250000 0.000000 0.500000
O 0.250000 0.000000 0.590909
O 0.253501 0.991639 0.681876
O 0.250000 0.500000 0.500000
O 0.250000 0.500000 0.590909

O 0.253230 0.492158 0.681733
O 0.750000 0.750000 0.545455
O 0.750616 0.748715 0.636241
O 0.750000 0.250000 0.545455
O 0.751092 0.248601 0.636294
O 0.250000 0.750000 0.545455
O 0.251485 0.748726 0.636241
O 0.250000 0.250000 0.545455
O 0.251349 0.248605 0.636289
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
O 0.507712 0.746432 0.682439
O 0.500000 0.250000 0.500000
O 0.500000 0.250000 0.590909
O 0.507005 0.246649 0.681630
O 0.000000 0.750000 0.500000
O 0.000000 0.750000 0.590909
O 0.007657 0.746734 0.681820
O 0.000000 0.250000 0.500000
O 0.000000 0.250000 0.590909
O 0.007939 0.246977 0.681652
O 0.759070 0.987592 0.227483
O 0.753099 0.486061 0.228479
O 0.247239 0.986697 0.227597
O 0.251750 0.486413 0.228446
O 0.754424 0.748247 0.271909
O 0.751028 0.245607 0.273032
O 0.247805 0.747439 0.271877
O 0.253035 0.245806 0.272974
O 0.501544 0.743750 0.228489
O 0.511372 0.241136 0.227301
O 0.000917 0.741893 0.225217
O 0.010568 0.243604 0.227753
O 0.357728 0.738631 0.186096
O 0.644044 0.739571 0.186004
O 0.750000 0.000000 0.409091
O 0.752598 0.991945 0.318185
O 0.750000 0.500000 0.409091
O 0.752562 0.491931 0.318226
O 0.250000 0.000000 0.409091
O 0.253501 0.991639 0.318124
O 0.250000 0.500000 0.409091
O 0.253230 0.492158 0.318267
O 0.750000 0.750000 0.454545
O 0.750616 0.748715 0.363759
O 0.750000 0.250000 0.454545

O 0.751092 0.248601 0.363706
O 0.250000 0.750000 0.454545
O 0.251485 0.748726 0.363759
O 0.250000 0.250000 0.454545
O 0.251349 0.248605 0.363711
O 0.500000 0.750000 0.409091
O 0.507712 0.746432 0.317561
O 0.500000 0.250000 0.409091
O 0.507005 0.246649 0.318370
O 0.000000 0.750000 0.409091
O 0.007657 0.746734 0.318180
O 0.000000 0.250000 0.409091
O 0.007939 0.246977 0.318348

Structure 30. TiO_2-terminated $BaTiO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.07335600
_cell_length_b   8.07335600
_cell_length_c   44.40346100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.497665  0.498815  0.271799
  Ba  0.997520  0.998831  0.271802
  Ba  0.997719  0.492763  0.272825
  Ba  0.497760  0.992749  0.272829
  Ba  0.497776  0.498482  0.363814
  Ba  0.997785  0.998473  0.363815
  Ba  0.497896  0.997971  0.363908
  Ba  0.997905  0.497983  0.363909
  Ba  0.000000  0.000000  0.454545
  Ba  0.000000  0.500000  0.454545
  Ba  0.500000  0.000000  0.454545
  Ba  0.500000  0.500000  0.454545
  Ba  0.000000  0.000000  0.545455
  Ba  0.000000  0.500000  0.545455
  Ba  0.500000  0.000000  0.545455
  Ba  0.500000  0.500000  0.545455
  Ba  0.997905  0.497983  0.636091
  Ba  0.497896  0.997971  0.636092
  Ba  0.997785  0.998473  0.636185
  Ba  0.497776  0.498482  0.636186
  Ba  0.497760  0.992749  0.727171
  Ba  0.997719  0.492763  0.727175
  Ba  0.997520  0.998831  0.728198
  Ba  0.497665  0.498815  0.728201
  Ti  0.769669  0.731147  0.227489
  Ti  0.269720  0.231377  0.227518
  Ti  0.729111  0.231142  0.227546
  Ti  0.229062  0.731413  0.227574
  Ti  0.239804  0.238894  0.318017
  Ti  0.739816  0.738832  0.318017
  Ti  0.237896  0.739196  0.318066
  Ti  0.737910  0.239147  0.318071
  Ti  0.250000  0.250000  0.409091
```

Ti 0.250000 0.750000 0.409091
Ti 0.750000 0.250000 0.409091
Ti 0.750000 0.750000 0.409091
Ti 0.250000 0.250000 0.500000
Ti 0.250000 0.750000 0.500000
Ti 0.750000 0.250000 0.500000
Ti 0.750000 0.750000 0.500000
Ti 0.250000 0.250000 0.590909
Ti 0.250000 0.750000 0.590909
Ti 0.750000 0.250000 0.590909
Ti 0.750000 0.750000 0.590909
Ti 0.737910 0.239147 0.681929
Ti 0.237896 0.739196 0.681934
Ti 0.239804 0.238894 0.681983
Ti 0.739816 0.738832 0.681983
Ti 0.229062 0.731413 0.772426
Ti 0.729111 0.231142 0.772453
Ti 0.269720 0.231377 0.772482
Ti 0.769669 0.731147 0.772511
C 0.499345 0.759053 0.198630
C 0.999470 0.259034 0.198631
C 0.999470 0.259034 0.801369
C 0.499345 0.759053 0.801370
O 0.642493 0.758456 0.186729
O 0.142697 0.258933 0.186758
O 0.856254 0.258422 0.186759
O 0.356051 0.758987 0.186787
O 0.499393 0.259546 0.225602
O 0.999356 0.759579 0.225610
O 0.754633 0.512841 0.228922
O 0.743782 0.012706 0.228942
O 0.254525 0.013053 0.228968
O 0.243869 0.512964 0.228982
O 0.499512 0.755529 0.229197
O 0.999456 0.255554 0.229198
O 0.746789 0.253783 0.272314
O 0.246774 0.754031 0.272336
O 0.754823 0.753660 0.272401
O 0.254866 0.253914 0.272416
O 0.007594 0.253507 0.317780
O 0.507614 0.753483 0.317783
O 0.252955 0.508597 0.318183
O 0.752952 0.008517 0.318183
O 0.752659 0.508008 0.318220
O 0.252653 0.008098 0.318221
O 0.506804 0.253660 0.318291

O 0.006767 0.753673 0.318292
O 0.250861 0.251587 0.363687
O 0.750860 0.751528 0.363687
O 0.751233 0.251572 0.363701
O 0.251226 0.751627 0.363705
O 0.250000 0.500000 0.409091
O 0.750000 0.000000 0.409091
O 0.250000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.000000 0.250000 0.409091
O 0.000000 0.750000 0.409091
O 0.500000 0.750000 0.409091
O 0.500000 0.250000 0.409091
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O 0.750000 0.750000 0.454545
O 0.250000 0.750000 0.454545
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O 0.250000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
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O 0.500000 0.750000 0.500000
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O 0.250000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.750000 0.750000 0.545455
O 0.250000 0.000000 0.590909
O 0.250000 0.500000 0.590909
O 0.750000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.000000 0.250000 0.590909
O 0.000000 0.750000 0.590909
O 0.500000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.251226 0.751627 0.636294
O 0.751233 0.251572 0.636299
O 0.250861 0.251587 0.636313
O 0.750860 0.751528 0.636313
O 0.006767 0.753673 0.681708
O 0.506804 0.253660 0.681709
O 0.252653 0.008098 0.681779
O 0.752659 0.508008 0.681780
O 0.752952 0.008517 0.681817

O 0.252955 0.508597 0.681817
O 0.507614 0.753483 0.682217
O 0.007594 0.253507 0.682220
O 0.254866 0.253914 0.727584
O 0.754823 0.753660 0.727599
O 0.246774 0.754031 0.727664
O 0.746789 0.253783 0.727686
O 0.999456 0.255554 0.770802
O 0.499512 0.755529 0.770803
O 0.243869 0.512964 0.771018
O 0.254525 0.013053 0.771032
O 0.743782 0.012706 0.771058
O 0.754633 0.512841 0.771078
O 0.999356 0.759579 0.774390
O 0.499393 0.259546 0.774398
O 0.356051 0.758987 0.813213
O 0.856254 0.258422 0.813241
O 0.142697 0.258933 0.813242
O 0.642493 0.758456 0.813271

Structure 31. ZrO_2-terminated $BaZrO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.000000  0.000000  0.545455
  Ba  0.999663  0.000202  0.636864
  Ba  0.998984  0.000414  0.729915
  Ba  0.000000  0.500000  0.545455
  Ba  0.999626  0.500243  0.636882
  Ba  0.998973  0.500429  0.729914
  Ba  0.500000  0.000000  0.545455
  Ba  0.499629  0.000186  0.636870
  Ba  0.498952  0.000403  0.729912
  Ba  0.500000  0.500000  0.545455
  Ba  0.499671  0.500141  0.636869
  Ba  0.498984  0.500414  0.729906
  Ba  0.000000  0.000000  0.454545
  Ba  0.999663  0.000202  0.363136
  Ba  0.998984  0.000414  0.270085
  Ba  0.000000  0.500000  0.454545
  Ba  0.999626  0.500243  0.363118
  Ba  0.998973  0.500429  0.270086
  Ba  0.500000  0.000000  0.454545
  Ba  0.499629  0.000186  0.363130
  Ba  0.498952  0.000403  0.270088
  Ba  0.500000  0.500000  0.454545
  Ba  0.499671  0.500141  0.363131
  Ba  0.498984  0.500414  0.270094
  Zr  0.250000  0.250000  0.500000
  Zr  0.250000  0.250000  0.590909
  Zr  0.249369  0.250299  0.681444
  Zr  0.248961  0.250433  0.770418
  Zr  0.250000  0.750000  0.500000
  Zr  0.250000  0.750000  0.590909
  Zr  0.249353  0.750319  0.681445
  Zr  0.248938  0.750409  0.770424
  Zr  0.750000  0.250000  0.500000
```

Zr 0.750000 0.250000 0.590909
Zr 0.749359 0.250281 0.681444
Zr 0.748946 0.250408 0.770417
Zr 0.750000 0.750000 0.500000
Zr 0.750000 0.750000 0.590909
Zr 0.749344 0.750298 0.681445
Zr 0.748918 0.750408 0.770423
Zr 0.250000 0.250000 0.409091
Zr 0.249369 0.250299 0.318556
Zr 0.248961 0.250433 0.229582
Zr 0.250000 0.750000 0.409091
Zr 0.249353 0.750319 0.318555
Zr 0.248938 0.750409 0.229576
Zr 0.750000 0.250000 0.409091
Zr 0.749359 0.250281 0.318556
Zr 0.748946 0.250408 0.229583
Zr 0.750000 0.750000 0.409091
Zr 0.749344 0.750298 0.318555
Zr 0.748918 0.750408 0.229577
O 0.250000 0.000000 0.500000
O 0.250000 0.000000 0.590909
O 0.245272 0.000308 0.681701
O 0.249391 0.000446 0.771309
O 0.250000 0.500000 0.500000
O 0.250000 0.500000 0.590909
O 0.253321 0.500310 0.681674
O 0.248391 0.500443 0.771322
O 0.750000 0.000000 0.500000
O 0.750000 0.000000 0.590909
O 0.753320 0.000288 0.681667
O 0.748419 0.000422 0.771309
O 0.750000 0.500000 0.500000
O 0.750000 0.500000 0.590909
O 0.745252 0.500292 0.681703
O 0.749405 0.500416 0.771318
O 0.250000 0.250000 0.545455
O 0.249679 0.250093 0.636497
O 0.249159 0.250432 0.727639
O 0.250000 0.750000 0.545455
O 0.249557 0.750245 0.636498
O 0.249131 0.750345 0.727644
O 0.750000 0.250000 0.545455
O 0.749576 0.250233 0.636497
O 0.749079 0.250339 0.727638
O 0.750000 0.750000 0.545455
O 0.749663 0.750064 0.636498

O 0.749024 0.750369 0.727642
O 0.000000 0.250000 0.500000
O 0.000000 0.250000 0.590909
O 0.999337 0.254333 0.681691
O 0.998941 0.249953 0.771339
O 0.000000 0.750000 0.500000
O 0.000000 0.750000 0.590909
O 0.999320 0.746306 0.681706
O 0.998914 0.750939 0.771360
O 0.500000 0.250000 0.500000
O 0.500000 0.250000 0.590909
O 0.499337 0.246261 0.681701
O 0.498940 0.250943 0.771359
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
O 0.499320 0.754376 0.681690
O 0.498913 0.749954 0.771374
O 0.250000 0.000000 0.409091
O 0.245272 0.000308 0.318299
O 0.249391 0.000446 0.228691
O 0.250000 0.500000 0.409091
O 0.253321 0.500310 0.318326
O 0.248391 0.500443 0.228678
O 0.750000 0.000000 0.409091
O 0.753320 0.000288 0.318333
O 0.748419 0.000422 0.228691
O 0.750000 0.500000 0.409091
O 0.745252 0.500292 0.318297
O 0.749405 0.500416 0.228682
O 0.250000 0.250000 0.454545
O 0.249679 0.250093 0.363503
O 0.249159 0.250432 0.272361
O 0.250000 0.750000 0.454545
O 0.249557 0.750245 0.363502
O 0.249131 0.750345 0.272356
O 0.750000 0.250000 0.454545
O 0.749576 0.250233 0.363503
O 0.749079 0.250339 0.272362
O 0.750000 0.750000 0.454545
O 0.749663 0.750064 0.363502
O 0.749024 0.750369 0.272358
O 0.000000 0.250000 0.409091
O 0.999337 0.254333 0.318309
O 0.998941 0.249953 0.228661
O 0.000000 0.750000 0.409091
O 0.999320 0.746306 0.318294

O 0.998914 0.750939 0.228640
O 0.500000 0.250000 0.409091
O 0.499337 0.246261 0.318299
O 0.498940 0.250943 0.228641
O 0.500000 0.750000 0.409091
O 0.499320 0.754376 0.318310
O 0.498913 0.749954 0.228626

Structure 32. ZrO_2-terminated $BaZrO_3$ slab at Θ=0.25 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.499669  0.500156  0.270880
  Ba  0.499662  0.000838  0.270937
  Ba  0.999667  0.495692  0.271865
  Ba  0.999669  0.005441  0.271896
  Ba  0.499866  0.502364  0.363300
  Ba  0.499865  0.998257  0.363316
  Ba  0.999866  0.502414  0.363320
  Ba  0.999868  0.998066  0.363352
  Ba  0.000000  0.000000  0.454545
  Ba  0.000000  0.500000  0.454545
  Ba  0.500000  0.000000  0.454545
  Ba  0.500000  0.500000  0.454545
  Ba  0.000000  0.000000  0.545455
  Ba  0.000000  0.500000  0.545455
  Ba  0.500000  0.000000  0.545455
  Ba  0.500000  0.500000  0.545455
  Ba  0.999868  0.998066  0.636648
  Ba  0.999866  0.502414  0.636680
  Ba  0.499865  0.998257  0.636684
  Ba  0.499866  0.502364  0.636700
  Ba  0.999669  0.005441  0.728104
  Ba  0.999667  0.495692  0.728135
  Ba  0.499662  0.000838  0.729063
  Ba  0.499669  0.500156  0.729120
  Zr  0.765626  0.750552  0.227934
  Zr  0.233644  0.750541  0.227935
  Zr  0.249096  0.250484  0.230141
  Zr  0.750212  0.250475  0.230142
  Zr  0.250510  0.750394  0.317802
  Zr  0.749002  0.750397  0.317802
  Zr  0.250229  0.250393  0.318969
  Zr  0.749284  0.250391  0.318969
  Zr  0.250000  0.250000  0.409091
```

Zr 0.250000 0.750000 0.409091
Zr 0.750000 0.250000 0.409091
Zr 0.750000 0.750000 0.409091
Zr 0.250000 0.250000 0.500000
Zr 0.250000 0.750000 0.500000
Zr 0.750000 0.250000 0.500000
Zr 0.750000 0.750000 0.500000
Zr 0.250000 0.250000 0.590909
Zr 0.250000 0.750000 0.590909
Zr 0.750000 0.250000 0.590909
Zr 0.750000 0.750000 0.590909
Zr 0.250229 0.250393 0.681031
Zr 0.749284 0.250391 0.681031
Zr 0.250510 0.750394 0.682198
Zr 0.749002 0.750397 0.682198
Zr 0.750212 0.250475 0.769858
Zr 0.249096 0.250484 0.769859
Zr 0.233644 0.750541 0.772065
Zr 0.765626 0.750552 0.772066
C 0.499617 0.752565 0.197733
C 0.499617 0.752565 0.802267
O 0.634582 0.753110 0.186076
O 0.364641 0.753150 0.186079
O 0.499624 0.751049 0.226973
O 0.999644 0.250503 0.229170
O 0.499646 0.251064 0.229465
O 0.999631 0.751460 0.229587
O 0.247596 0.501730 0.230566
O 0.751661 0.501733 0.230582
O 0.751145 0.000144 0.230782
O 0.248123 0.000146 0.230792
O 0.262095 0.750239 0.271949
O 0.737295 0.750315 0.271950
O 0.247852 0.251154 0.272947
O 0.751564 0.251081 0.272948
O 0.999751 0.746362 0.316811
O 0.499751 0.246064 0.318046
O 0.999752 0.254467 0.318343
O 0.245097 0.000516 0.318457
O 0.754352 0.000517 0.318470
O 0.746042 0.500268 0.318543
O 0.253411 0.500268 0.318556
O 0.499752 0.754622 0.319188
O 0.752625 0.750246 0.363404
O 0.247114 0.750289 0.363405
O 0.250571 0.250075 0.363659

O 0.749169 0.250122 0.363659
O 0.250000 0.000000 0.409091
O 0.250000 0.500000 0.409091
O 0.750000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.000000 0.250000 0.409091
O 0.000000 0.750000 0.409091
O 0.500000 0.250000 0.409091
O 0.500000 0.750000 0.409091
O 0.250000 0.250000 0.454545
O 0.750000 0.250000 0.454545
O 0.250000 0.750000 0.454545
O 0.750000 0.750000 0.454545
O 0.250000 0.000000 0.500000
O 0.250000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.000000 0.250000 0.500000
O 0.000000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.250000 0.250000 0.545455
O 0.250000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.750000 0.750000 0.545455
O 0.250000 0.000000 0.590909
O 0.250000 0.500000 0.590909
O 0.750000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.000000 0.250000 0.590909
O 0.000000 0.750000 0.590909
O 0.500000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.250571 0.250075 0.636341
O 0.749169 0.250122 0.636341
O 0.247114 0.750289 0.636595
O 0.752625 0.750246 0.636596
O 0.499752 0.754622 0.680812
O 0.253411 0.500268 0.681444
O 0.746042 0.500268 0.681457
O 0.754352 0.000517 0.681530
O 0.245097 0.000516 0.681543
O 0.999752 0.254467 0.681657
O 0.499751 0.246064 0.681954
O 0.999751 0.746362 0.683189
O 0.751564 0.251081 0.727052

O 0.247852 0.251154 0.727053
O 0.737295 0.750315 0.728050
O 0.262095 0.750239 0.728051
O 0.248123 0.000146 0.769208
O 0.751145 0.000144 0.769218
O 0.751661 0.501733 0.769418
O 0.247596 0.501730 0.769434
O 0.999631 0.751460 0.770413
O 0.499646 0.251064 0.770535
O 0.999644 0.250503 0.770830
O 0.499624 0.751049 0.773027
O 0.364641 0.753150 0.813921
O 0.634582 0.753110 0.813924

Structure 33. ZrO_2-terminated $BaZrO_3$ slab at Θ=0.50 CO_2 coverage

```
_cell_length_a   8.51149400
_cell_length_b   8.51149400
_cell_length_c   46.81321300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.999642  0.003972  0.272546
  Ba  0.499642  0.503972  0.272546
  Ba  0.999640  0.494615  0.272636
  Ba  0.499641  0.994615  0.272636
  Ba  0.999832  0.000166  0.363531
  Ba  0.999830  0.500052  0.363531
  Ba  0.499829  0.000051  0.363531
  Ba  0.499831  0.500164  0.363531
  Ba  0.000000  0.000000  0.454545
  Ba  0.000000  0.500000  0.454545
  Ba  0.500000  0.000000  0.454545
  Ba  0.500000  0.500000  0.454545
  Ba  0.000000  0.000000  0.545455
  Ba  0.000000  0.500000  0.545455
  Ba  0.500000  0.000000  0.545455
  Ba  0.500000  0.500000  0.545455
  Ba  0.999832  0.000166  0.636469
  Ba  0.999830  0.500052  0.636469
  Ba  0.499829  0.000051  0.636469
  Ba  0.499831  0.500164  0.636469
  Ba  0.999640  0.494615  0.727364
  Ba  0.499641  0.994615  0.727364
  Ba  0.999642  0.003972  0.727454
  Ba  0.499642  0.503972  0.727454
  Zr  0.265291  0.247393  0.228575
  Zr  0.765288  0.747393  0.228575
  Zr  0.233976  0.747390  0.228576
  Zr  0.733978  0.247389  0.228576
  Zr  0.249456  0.249988  0.318278
  Zr  0.749456  0.749987  0.318278
  Zr  0.249931  0.749989  0.318279
  Zr  0.749932  0.249988  0.318279
  Zr  0.250000  0.250000  0.409091
```

Zr 0.250000 0.750000 0.409091
Zr 0.750000 0.250000 0.409091
Zr 0.750000 0.750000 0.409091
Zr 0.250000 0.250000 0.500000
Zr 0.250000 0.750000 0.500000
Zr 0.750000 0.250000 0.500000
Zr 0.750000 0.750000 0.500000
Zr 0.250000 0.250000 0.590909
Zr 0.250000 0.750000 0.590909
Zr 0.750000 0.250000 0.590909
Zr 0.750000 0.750000 0.590909
Zr 0.249931 0.749989 0.681721
Zr 0.749932 0.249988 0.681721
Zr 0.249456 0.249988 0.681722
Zr 0.749456 0.749987 0.681722
Zr 0.233976 0.747390 0.771424
Zr 0.733978 0.247389 0.771424
Zr 0.765288 0.747393 0.771425
Zr 0.265291 0.247393 0.771425
C 0.499622 0.751806 0.198637
C 0.999617 0.251800 0.198637
C 0.999617 0.251800 0.801363
C 0.499622 0.751806 0.801363
O 0.134613 0.251797 0.187087
O 0.634609 0.751804 0.187088
O 0.364625 0.751817 0.187088
O 0.864636 0.251810 0.187088
O 0.999626 0.251142 0.227981
O 0.499623 0.751143 0.227982
O 0.499632 0.252795 0.230874
O 0.999632 0.752795 0.230875
O 0.248568 0.501408 0.231903
O 0.748568 0.001407 0.231903
O 0.250709 0.001409 0.231907
O 0.750709 0.501408 0.231907
O 0.235514 0.250639 0.272589
O 0.735512 0.750638 0.272589
O 0.263818 0.750607 0.272590
O 0.763816 0.250607 0.272590
O 0.999675 0.746302 0.316732
O 0.499675 0.246301 0.316733
O 0.245639 0.000133 0.318635
O 0.745639 0.500133 0.318635
O 0.253568 0.500134 0.318643
O 0.753568 0.000133 0.318644
O 0.999677 0.254207 0.319330

O 0.499677 0.754208 0.319330
O 0.252891 0.250012 0.363571
O 0.752892 0.750010 0.363571
O 0.246776 0.750053 0.363572
O 0.746778 0.250053 0.363572
O 0.250000 0.500000 0.409091
O 0.750000 0.000000 0.409091
O 0.250000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.000000 0.250000 0.409091
O 0.000000 0.750000 0.409091
O 0.500000 0.750000 0.409091
O 0.500000 0.250000 0.409091
O 0.750000 0.250000 0.454545
O 0.750000 0.750000 0.454545
O 0.250000 0.750000 0.454545
O 0.250000 0.250000 0.454545
O 0.250000 0.000000 0.500000
O 0.250000 0.500000 0.500000
O 0.750000 0.000000 0.500000
O 0.750000 0.500000 0.500000
O 0.000000 0.250000 0.500000
O 0.000000 0.750000 0.500000
O 0.500000 0.250000 0.500000
O 0.500000 0.750000 0.500000
O 0.250000 0.250000 0.545455
O 0.250000 0.750000 0.545455
O 0.750000 0.250000 0.545455
O 0.750000 0.750000 0.545455
O 0.250000 0.000000 0.590909
O 0.250000 0.500000 0.590909
O 0.750000 0.000000 0.590909
O 0.750000 0.500000 0.590909
O 0.000000 0.250000 0.590909
O 0.000000 0.750000 0.590909
O 0.500000 0.250000 0.590909
O 0.500000 0.750000 0.590909
O 0.246776 0.750053 0.636428
O 0.746778 0.250053 0.636428
O 0.252891 0.250012 0.636429
O 0.752892 0.750010 0.636429
O 0.999677 0.254207 0.680670
O 0.499677 0.754208 0.680670
O 0.753568 0.000133 0.681356
O 0.253568 0.500134 0.681357
O 0.245639 0.000133 0.681365

O 0.745639 0.500133 0.681365
O 0.499675 0.246301 0.683267
O 0.999675 0.746302 0.683268
O 0.263818 0.750607 0.727410
O 0.763816 0.250607 0.727410
O 0.235514 0.250639 0.727411
O 0.735512 0.750638 0.727411
O 0.250709 0.001409 0.768093
O 0.750709 0.501408 0.768093
O 0.748568 0.001407 0.768097
O 0.248568 0.501408 0.768097
O 0.999632 0.752795 0.769125
O 0.499632 0.252795 0.769126
O 0.499623 0.751143 0.772018
O 0.999626 0.251142 0.772019
O 0.634609 0.751804 0.812912
O 0.364625 0.751817 0.812912
O 0.864636 0.251810 0.812912
O 0.134613 0.251797 0.812913

Structure 34. HfO_2-terminated $BaHfO_3$ slab at Θ=0.00 CO_2 coverage

```
_cell_length_a   8.41088800
_cell_length_b   8.41088800
_cell_length_c   46.25988800
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  Ba  0.000000  0.000000  0.545455
  Ba  0.000716  0.000328  0.636749
  Ba  0.001812  0.000894  0.729555
  Ba  0.000000  0.500000  0.545455
  Ba  0.000699  0.500363  0.636737
  Ba  0.001812  0.500865  0.729553
  Ba  0.500000  0.000000  0.545455
  Ba  0.500765  0.000319  0.636752
  Ba  0.501739  0.000887  0.729556
  Ba  0.500000  0.500000  0.545455
  Ba  0.500762  0.500386  0.636741
  Ba  0.501828  0.500825  0.729554
  Ba  0.000000  0.000000  0.454545
  Ba  0.000716  0.000328  0.363251
  Ba  0.001812  0.000894  0.270445
  Ba  0.000000  0.500000  0.454545
  Ba  0.000699  0.500363  0.363263
  Ba  0.001812  0.500865  0.270447
  Ba  0.500000  0.000000  0.454545
  Ba  0.500765  0.000319  0.363248
  Ba  0.501739  0.000887  0.270444
  Ba  0.500000  0.500000  0.454545
  Ba  0.500762  0.500386  0.363259
  Ba  0.501828  0.500825  0.270446
  Hf  0.250000  0.250000  0.500000
  Hf  0.250000  0.250000  0.590909
  Hf  0.251230  0.250593  0.681395
  Hf  0.251854  0.250933  0.770191
  Hf  0.250000  0.750000  0.500000
  Hf  0.250000  0.750000  0.590909
  Hf  0.251243  0.750573  0.681400
  Hf  0.251869  0.750862  0.770190
  Hf  0.750000  0.250000  0.500000
```

Hf 0.750000 0.250000 0.590909
Hf 0.751234 0.250592 0.681401
Hf 0.751874 0.250852 0.770194
Hf 0.750000 0.750000 0.500000
Hf 0.750000 0.750000 0.590909
Hf 0.751236 0.750606 0.681407
Hf 0.751846 0.750925 0.770193
Hf 0.250000 0.250000 0.409091
Hf 0.251230 0.250593 0.318605
Hf 0.251854 0.250933 0.229809
Hf 0.250000 0.750000 0.409091
Hf 0.251243 0.750573 0.318600
Hf 0.251869 0.750862 0.229810
Hf 0.750000 0.250000 0.409091
Hf 0.751234 0.250592 0.318599
Hf 0.751874 0.250852 0.229806
Hf 0.750000 0.750000 0.409091
Hf 0.751236 0.750606 0.318593
Hf 0.751846 0.750925 0.229807
O 0.250000 0.000000 0.500000
O 0.250000 0.000000 0.590909
O 0.252034 0.000568 0.681729
O 0.251754 0.000896 0.771535
O 0.250000 0.500000 0.500000
O 0.250000 0.500000 0.590909
O 0.250369 0.500572 0.681676
O 0.251989 0.500893 0.771593
O 0.750000 0.000000 0.500000
O 0.750000 0.000000 0.590909
O 0.750362 0.000583 0.681671
O 0.751974 0.000897 0.771610
O 0.750000 0.500000 0.500000
O 0.750000 0.500000 0.590909
O 0.752014 0.500585 0.681738
O 0.751749 0.500893 0.771532
O 0.250000 0.250000 0.545455
O 0.250662 0.250217 0.636432
O 0.251476 0.250880 0.727460
O 0.250000 0.750000 0.545455
O 0.250643 0.750407 0.636433
O 0.251597 0.750564 0.727458
O 0.750000 0.250000 0.545455
O 0.750650 0.250431 0.636434
O 0.751593 0.250530 0.727463
O 0.750000 0.750000 0.545455
O 0.750682 0.750203 0.636435

O 0.751489 0.750958 0.727462
O 0.000000 0.250000 0.500000
O 0.000000 0.250000 0.590909
O 0.001203 0.249739 0.681696
O 0.001869 0.251010 0.771583
O 0.000000 0.750000 0.500000
O 0.000000 0.750000 0.590909
O 0.001211 0.751384 0.681714
O 0.001866 0.750774 0.771560
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O 0.500000 0.250000 0.590909
O 0.501208 0.251409 0.681706
O 0.501865 0.250785 0.771561
O 0.500000 0.750000 0.500000
O 0.500000 0.750000 0.590909
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O 0.501863 0.751007 0.771574
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O 0.251754 0.000896 0.228465
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O 0.250369 0.500572 0.318324
O 0.251989 0.500893 0.228407
O 0.750000 0.000000 0.409091
O 0.750362 0.000583 0.318329
O 0.751974 0.000897 0.228390
O 0.750000 0.500000 0.409091
O 0.752014 0.500585 0.318262
O 0.751749 0.500893 0.228468
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O 0.250662 0.250217 0.363568
O 0.251476 0.250880 0.272540
O 0.250000 0.750000 0.454545
O 0.250643 0.750407 0.363567
O 0.251597 0.750564 0.272542
O 0.750000 0.250000 0.454545
O 0.750650 0.250431 0.363566
O 0.751593 0.250530 0.272537
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O 0.750682 0.750203 0.363565
O 0.751489 0.750958 0.272538
O 0.000000 0.250000 0.409091
O 0.001203 0.249739 0.318303
O 0.001869 0.251010 0.228417
O 0.000000 0.750000 0.409091
O 0.001211 0.751384 0.318286

O 0.001866 0.750774 0.228440
O 0.500000 0.250000 0.409091
O 0.501208 0.251409 0.318294
O 0.501865 0.250785 0.228439
O 0.500000 0.750000 0.409091
O 0.501214 0.749738 0.318307
O 0.501863 0.751007 0.228426

Structure 35. HfO_2-terminated $BaHfO_3$ slab at Θ=0.25 CO_2 coverage

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_cell_length_b   8.41088800
_cell_length_c   46.25988800
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
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  Ba  0.500888  0.001191  0.271129
  Ba  0.000891  0.497214  0.271883
  Ba  0.000890  0.004366  0.271895
  Ba  0.500348  0.502010  0.363383
  Ba  0.000345  0.501977  0.363386
  Ba  0.000346  0.998611  0.363387
  Ba  0.500346  0.998584  0.363387
  Ba  0.000000  0.000000  0.454545
  Ba  0.000000  0.500000  0.454545
  Ba  0.500000  0.000000  0.454545
  Ba  0.500000  0.500000  0.454545
  Ba  0.000000  0.000000  0.545455
  Ba  0.000000  0.500000  0.545455
  Ba  0.500000  0.000000  0.545455
  Ba  0.500000  0.500000  0.545455
  Ba  0.000346  0.998611  0.636613
  Ba  0.500346  0.998584  0.636613
  Ba  0.000345  0.501977  0.636614
  Ba  0.500348  0.502010  0.636617
  Ba  0.000890  0.004366  0.728105
  Ba  0.000891  0.497214  0.728117
  Ba  0.500888  0.001191  0.728871
  Ba  0.500890  0.500432  0.728900
  Hf  0.234747  0.750857  0.227838
  Hf  0.767263  0.750869  0.227849
  Hf  0.250438  0.250834  0.230321
  Hf  0.751388  0.250836  0.230324
  Hf  0.251088  0.750518  0.317886
  Hf  0.750145  0.750522  0.317888
  Hf  0.251035  0.250544  0.318940
  Hf  0.750155  0.250544  0.318940
  Hf  0.250000  0.250000  0.409091
```

Hf 0.250000 0.750000 0.409091
Hf 0.750000 0.250000 0.409091
Hf 0.750000 0.750000 0.409091
Hf 0.250000 0.250000 0.500000
Hf 0.250000 0.750000 0.500000
Hf 0.750000 0.250000 0.500000
Hf 0.750000 0.750000 0.500000
Hf 0.250000 0.250000 0.590909
Hf 0.250000 0.750000 0.590909
Hf 0.750000 0.250000 0.590909
Hf 0.750000 0.750000 0.590909
Hf 0.251035 0.250544 0.681060
Hf 0.750155 0.250544 0.681060
Hf 0.750145 0.750522 0.682112
Hf 0.251088 0.750518 0.682114
Hf 0.751388 0.250836 0.769676
Hf 0.250438 0.250834 0.769679
Hf 0.767263 0.750869 0.772151
Hf 0.234747 0.750857 0.772162
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C 0.501097 0.752135 0.802333
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O 0.637992 0.752439 0.186049
O 0.501033 0.751239 0.227339
O 0.001006 0.750765 0.227548
O 0.500931 0.250696 0.229114
O 0.000930 0.251007 0.229127
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O 0.752355 0.501349 0.230065
O 0.249227 0.000528 0.230162
O 0.752706 0.000548 0.230169
O 0.256487 0.750573 0.271991
O 0.745230 0.750612 0.271998
O 0.250229 0.250947 0.273082
O 0.751270 0.250925 0.273085
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O 0.500585 0.250704 0.318201
O 0.000588 0.250301 0.318313
O 0.500605 0.750287 0.318405
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O 0.750478 0.000643 0.318435
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O 0.250260 0.500411 0.318462
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O 0.751205 0.750309 0.363442
O 0.250564 0.250237 0.363700

O 0.750039 0.250251 0.363701
O 0.250000 0.000000 0.409091
O 0.250000 0.500000 0.409091
O 0.750000 0.000000 0.409091
O 0.750000 0.500000 0.409091
O 0.000000 0.250000 0.409091
O 0.000000 0.750000 0.409091
O 0.500000 0.250000 0.409091
O 0.500000 0.750000 0.409091
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O 0.250564 0.250237 0.636300
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O 0.750478 0.000643 0.681565
O 0.250686 0.000640 0.681571
O 0.500605 0.750287 0.681595
O 0.000588 0.250301 0.681687
O 0.500585 0.250704 0.681799
O 0.000611 0.750705 0.682535
O 0.751270 0.250925 0.726915

O 0.250229 0.250947 0.726918
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O 0.256487 0.750573 0.728009
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O 0.249227 0.000528 0.769838
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O 0.249569 0.501335 0.769952
O 0.000930 0.251007 0.770873
O 0.500931 0.250696 0.770886
O 0.001006 0.750765 0.772452
O 0.501033 0.751239 0.772661
O 0.637992 0.752439 0.813951
O 0.364241 0.752448 0.813966

Structure 36. HfO_2-terminated $BaHfO_3$ slab at Θ=0.50 CO_2 coverage

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_cell_length_b   8.41088800
_cell_length_c   46.25988800
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_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_space_group_name_H-M   'P 1'
loop_
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
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  Ba  0.500932  0.503891  0.272503
  Ba  0.500927  0.997266  0.272507
  Ba  0.000925  0.497264  0.272508
  Ba  0.000482  0.000336  0.363545
  Ba  0.500482  0.500335  0.363546
  Ba  0.000470  0.500177  0.363550
  Ba  0.500469  0.000177  0.363550
  Ba  0.000000  0.000000  0.454545
  Ba  0.000000  0.500000  0.454545
  Ba  0.500000  0.000000  0.454545
  Ba  0.500000  0.500000  0.454545
  Ba  0.000000  0.000000  0.545455
  Ba  0.000000  0.500000  0.545455
  Ba  0.500000  0.000000  0.545455
  Ba  0.500000  0.500000  0.545455
  Ba  0.000470  0.500177  0.636450
  Ba  0.500469  0.000177  0.636450
  Ba  0.500482  0.500335  0.636454
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  Ba  0.000925  0.497264  0.727492
  Ba  0.500927  0.997266  0.727493
  Ba  0.000930  0.003889  0.727497
  Ba  0.500932  0.503891  0.727497
  Hf  0.735172  0.250586  0.228417
  Hf  0.235168  0.750588  0.228418
  Hf  0.266724  0.250599  0.228422
  Hf  0.766722  0.750600  0.228422
  Hf  0.750837  0.250447  0.318282
  Hf  0.250836  0.750448  0.318283
  Hf  0.250724  0.250451  0.318284
  Hf  0.750723  0.750450  0.318284
  Hf  0.250000  0.250000  0.409091
```

Hf 0.250000 0.750000 0.409091
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Hf 0.750000 0.750000 0.409091
Hf 0.250000 0.250000 0.500000
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Hf 0.750837 0.250447 0.681718
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Hf 0.235168 0.750588 0.771582
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C 0.500977 0.750938 0.198426
C 0.500977 0.750938 0.801574
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O 0.364080 0.750996 0.813090
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Reference

1. R. D. Shannon, *Acta Crystallographica Section A: Crystal Physics, Diffraction, Theoretical and General Crystallography*, 1976, **32**, 751-767.