Suppression of Surfaces States at Cubic Perovskite (001) Surfaces by CO$_2$ Adsorption

Kostiantyn V. Sopiha$^1$, Oleksandr I. Malyi$^2$, Clas Persson$^2$, Ping Wu$^1$

1 – Entropic Interface Group, Engineering Product Development, Singapore University of Technology and Design, 8 Somapah Road, 487372 Singapore, Singapore

2 – Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo, P. O. Box 1048 Blindern, NO-0316 Oslo, Norway

E-mails: oleksandrmalyi@gmail.com (O.I.M), wупing@sutd.edu.sg (W.P)

Abstract

By using first-principles approach, the interaction of CO$_2$ with (001) surfaces of six cubic ABO$_3$ perovskites (A = Ba, Sr and B = Ti, Zr, Hf) is studied in detail. We show that CO$_2$ adsorption results in the formation of highly stable CO$_3$-like complexes with similar geometries for all investigated compounds. This reaction leads to the suppression of the surfaces states, opening the band gaps of the slab systems up to the corresponding bulk energy limits. For most AO-terminated ABO$_3$(001) perovskite surfaces, a CO$_2$ coverage of 0.25 was found to be sufficient to fully suppress the surface states, whereas the same effect can only be achieved at 0.50 CO$_2$ coverage for the BO$_2$ terminations. The largest band gap modulation among the AO-terminated surfaces was found for SrHfO$_3$(001) and BaHfO$_3$(001), whereas the most profound effect among the BO$_2$ terminations was identified for SrTiO$_3$(001) and BaTiO$_3$(001). Based on these results and considering practical difficulties associated with measuring conductivity of highly resistive materials, TiO$_2$-terminated SrTiO$_3$(001) and BaTiO$_3$(001) were identified as the most prospective candidates for chemiresistive CO$_2$ sensing applications.

Keywords: perovskites, CO$_2$ adsorption, sensing mechanism, surface states, band gap modulation
Introduction

An early discovery of gas sensing features in metal-oxides\(^1\) has triggered an intensive search for functional materials having superior gas sensing characteristics.\(^2\-^4\) Despite this apparent success, in general, chemiresistive sensing of chemically inert gases remains practically difficult. Specifically, measuring CO\(_2\) concentration is currently performed using optical gas detectors, which are not well suited for mass-scale applications due to their high production cost imposed by the structural complexity.\(^5\) From the chemical perspective, a majority of classical sensing oxides are practically incapable of chemiresistive CO\(_2\) detection due to high stability of the CO\(_2\) molecule.\(^3\, ^4\, ^6\) In an attempt to overcome this obstacle, research focus has gradually shifted to alternative sensing materials, including various inorganic perovskites possessing prospective CO\(_2\) sensing characteristics.\(^7\-^17\)

The first efficient perovskite-based CO\(_2\) sensor was developed by Meyer \textit{et al.}, who discovered profound chemiresistive features of BaTiO\(_3\)-containing composites.\(^7\, ^8\) Since then, the optimized composition consisting of BaTiO\(_3\), CuO, and La\(_2\)O\(_3\) has long been the best-performing CO\(_2\) sensing material reported in the literature\(^4\, ^8\) until the recent development of BaSnO\(_3\)-based chemiresistor.\(^9\) To understand the sensing phenomenon, CO\(_2\) sensing properties of the BaTiO\(_3\)-CuO composites were examined by different authors.\(^18\-^26\) The studies revealed the formation of surface carbonate groups and proposed a CO\(_2\) sensing mechanism based on modulation of the electron energy levels at BaTiO\(_3\)/CuO heterointerfaces.\(^21\-^24\) Although this mechanism can explain chemiresistive response for the composites, it fails to justify experimental findings revealing CO\(_2\) sensing features of pristine\(^9\-^{11}\) and doped\(^12\-^{17}\) perovskites. Moreover, despite considerable progress achieved in the field, so far, reported values of the CO\(_2\) sensing response remain too low for practical use, highlighting a need for further research and functionalization of the perovskite-based sensing materials. The main obstacle for the further development, however, lays in a poor understanding of the adsorption chemistry of perovskite surfaces and its relation to the electrical conductivity.

To unveil the background surface chemistry of sensing, CO\(_2\) adsorption on stable (001) perovskite surfaces has been intensively investigated using first-principles methods. It was found that the CO\(_2\) adsorption results in the formation of highly stable CO\(_3\)-like complexes for all considered materials.\(^27\-^29\) Despite this knowledge, the exact mechanism on how the adsorption affects the surface conductivity has long remained uncertain. Recently, it has been demonstrated
that molecular chemisorption on $K_{1-y}Na_yTa_{1-x}Nb_xO_3(001)^{29, 30}$ and $SrTiO_3(001)^{31}$ results in the suppression of surface states emergent at their clean (001) facets. Since the existence of surface states can increase the surface conductivity\textsuperscript{32-34} and even contribute to the formation of 2-dimensional electron gas (2DEG),\textsuperscript{35} this suppression might be a long-missing link between the CO$_2$ adsorption and conductivity change during the sensing. However, since up to date the band gap modulation has only been explored for two representative perovskite materials, a wider family of the compounds should be considered to provide a better understanding and allow further generalization of the mechanism. Motivated by this, we investigated CO$_2$ interaction with (001) surfaces of different cubic ABO$_3$ perovskites (A = Ba, Sr and B = Ti, Zr, Hf) focusing on the adsorption-induced changes in the surface electronic properties. The material selection for this study was dictated by similar geometry and chemistry of the compounds, which can allow to reveal common adsorption trends for cubic perovskites by analyzing the roles played by different parameters (such as lattice constant, band gap, surface termination, etc.). The obtained results are expected to guide further optimization of the perovskite-based sensing materials for CO$_2$ sensing applications, catalysis, photocatalysis, and beyond.

**Methods**

The first-principles calculations were performed using Vienna \textit{ab initio} simulation package (VASP)\textsuperscript{36-38} utilizing Perdew-Burke-Ernzerhof (PBE) functional\textsuperscript{39} and projected augmented wave (PAW) pseudopotentials.\textsuperscript{40, 41} Barium 5s$^2$5p$^6$6s$^2$, strontium 4s$^2$4p$^6$5s$^2$, hafnium 5s$^2$5p$^6$5d$^6$6s$^2$, zirconium 4s$^2$4p$^6$4d$^2$5s$^2$, titanium 3s$^2$3p$^6$3d$^2$4s$^2$, oxygen 2s$^2$2p$^4$, and carbon 2s$^2$2p$^2$ were treated as valence electrons. The Brillouin-zone integrations were performed on $\Gamma$-centered 5×5×1 Monkhorst-Pack grids\textsuperscript{42} for ionic relaxations and the 10×10×1 grids for electronic structure calculations. The cutoff energies of 400 eV and atomic force threshold of 0.01 eV/Å were employed in all calculations. Since PBE is known to underestimate the band gap energies,\textsuperscript{43} electronic structures of the bulk and clean perovskite surfaces were also computed using hybrid Heyd-Scuseria-Ernzerhof (HSE06) functional with the default mixing coefficient of 0.25 for the exact exchange.\textsuperscript{44} The obtained results were analyzed using Vesta\textsuperscript{45} and pymatgen.\textsuperscript{46}

Bulk unit cells of cubic perovskites were relaxed imposing $Pm\bar{3}m$ symmetry. These phases has been found experimentally in all perovskite systems considered herein, although distorted phases are often the ground states.\textsuperscript{47} The optimized lattice parameters were used to construct model
slabs consisting of 13 atomic layers (6.5 unit cells) of the perovskites and about 20 Å (5.5 unit cells) of vacuum. Since previous first-principles\textsuperscript{48,49} and experimental\textsuperscript{50} observations revealed that (001) facets are the most stable for the perovskite systems, both the AO- and BO\textsubscript{2}-terminated ABO\textsubscript{3}(001) were investigated herein. Experimentally observed surface reconstructions were disregarded in this work due to their thermodynamic instability at ambient conditions.\textsuperscript{51-57} All atoms from five bulk-like middle layers were kept fixed during the relaxations to maintain the cubic symmetry of the deep atomic layers. In order to avoid dipole-dipole interaction due to the cell periodicity,\textsuperscript{58} CO\textsubscript{2} chemisorption on both sides of the symmetrical slabs was modeled. This model was validated for SrTiO\textsubscript{3}(001) surfaces in our recent study\textsuperscript{31} and compared to the alternative approaches\textsuperscript{27, 28} therein. Stability of CO\textsubscript{2} adsorption conformations was quantified by the adsorption energy calculated as $E_{\text{Ads}} = \left( E(\text{slab} + n \cdot \text{CO}_2) - E(\text{slab}) - n \cdot E(\text{CO}_2) \right) / n$, where $E(\text{slab} + n \cdot \text{CO}_2)$, $E(\text{slab})$, and $E(\text{CO}_2)$ are total energies of the slab containing $n$ adsorbed CO\textsubscript{2} molecules, clean slab relaxed after CO\textsubscript{2} desorption, and free CO\textsubscript{2} molecule, respectively. The CO\textsubscript{2} coverage ($\Theta$) was determined as the number of CO\textsubscript{2} molecules per unit cell of the surface. All local density of states (LDOS) for the slabs are presented in respect to the valence band maxima (VBM) of the corresponding bulk systems, where the alignment was performed based on average electrostatic potentials in cores of B-site cations in the bulk systems and three middle bulk-like atomic layers of the slabs. To demonstrate localization of the surface states, surface state densities were computed as charge densities for the states within energy limits from the conduction band minima (CBM) or VBM levels of the slabs to those of the corresponding bulk compounds.

**Results and discussion**

Before investigating an impact of CO\textsubscript{2} adsorption on electronic properties of the perovskite surfaces, we first established benchmarks for the bulk compounds, as summarized in Table S1. It was found that the considered compounds have lattice parameters varying from 3.95 Å for SrTiO\textsubscript{3} to 4.26 Å for BaZrO\textsubscript{3}, following the corresponding trends in the crystal ionic radii of the cations (Sr$^{2+}$: 1.32, Ba$^{2+}$: 1.49, Ti$^{4+}$: 0.745, Zr$^{4+}$: 0.86, and Hf$^{4+}$: 0.85 Å for the 6-coordinated ions).\textsuperscript{59} These systems have band gap energies between 1.69 and 3.74 eV computed on PBE level for BaTiO\textsubscript{3} and SrHfO\textsubscript{3}, respectively (see Fig. 1a). For both Sr- and Ba-containing perovskites, the energy gaps correlate with electronegativities of B-site cations (Ti: 1.54, Zr: 1.33, and Hf: 1.30 in Pauling
This trend reflects different localizations of $d$-like orbitals of B-site cations determining CBM positions in all considered compounds, as shown in Fig. S1.

As briefly mentioned in the methods section, the $Pm\overline{3}m$ crystal phases can undergo distortions at low temperatures. Although this tendency is largely constrained at the first-principles level by the fixation of bulk-like atomic layers (see methods), akin relaxations may still occur at the surfaces. Indeed, our first-principles analysis revealed that the ideal surfaces obtained from the ionic relaxation of as-cleaved slabs are metastable with respect to structural perturbation. Depending on the compound, several distortion patterns were found, as summarized in Fig. S2. The largest energy changes due to the distortion were computed for SrO-terminated SrZrO$_3$(001) and SrHfO$_3$(001), which were stabilized in respect to the ideal surfaces by 30.7 and 19.7 meV/Å$^2$, respectively (see Fig. S3). This behavior can be understood from the analysis of the Goldschmidt tolerance factor, which was developed to determine relative stability and distortion of perovskite structures. In this regard, the smallest tolerance factors were found for SrZrO$_3$ and SrHfO$_3$ (see Table S1), implying their low stability in cubic $Pm\overline{3}m$ phases near absolute zero. It should be noted that despite reaching the local minimum of energy, computed distortion patterns might be artificially stabilized by the imposed slab geometry constraints. However, accounting for the surface distortion is critical to separate adsorption-driven relaxations from those triggered by the broken symmetry. Therefore, the optimized slabs with the most stable distortion patterns were used as reference systems for the CO$_2$ adsorption energy calculations and addressed as clean surfaces henceforth.

By analyzing electronic properties of the stable (001) perovskite surfaces, we found that their band gaps are smaller compared to those of the corresponding bulk systems (see Fig. 1a), in agreement with previous reports. Although these energy gap reductions were observed for most investigated surfaces, the underlying mechanisms differ significantly among them. For the BO$_2$-terminated ABO$_3$(001), the effect is originated from the surface states emerging above the VBM of the bulk systems, as evident from the layer-resolved LDOS and projected surface state density shown in Fig. 1c,e on example of HfO$_2$-terminated SrHfO$_3$(001). These states are populated by $2p$-like electrons of O from the outermost BO$_2$ atomic layer. Importantly, we found that magnitude of the band gap reduction is not strongly dependent on the energy gap of the bulk system, falling within a range of 0.41-0.82 eV for all BO$_2$-terminated surfaces. In contrast, emerging surface states at the AO-terminated ABO$_3$(001) can have two different origins. In both
cases, the states emerge below CBM of the bulk compounds but can be localized either at the subsurface BO$_2$ or above the outermost AO atomic layer. The first scenario applies to SrO-terminated SrTiO$_3$(001), where vacant 3$d$-like orbitals from the subsurface Ti atoms (see Fig. 1f) reduce the band gap energy by 0.24 eV. Since this change is much smaller compared to that at the corresponding TiO$_2$-terminated surface (0.78 eV), the band gap reduction effect has less practical importance here. Similar behavior was also found for BaO-terminated BaTiO$_3$(001), where the surface state density at CBM implies formation of the surface states (see Fig. S5), but no reduction in the overall band gap energy of the slab system was observed, as reflected in Table S2. This result indicates that surface states at BaO-terminated BaTiO$_3$(001), if present, are within the error bar for electronic structure calculations and cannot alter the surface conductivity significantly. The second scenario leads to the band gap reductions of 0.27-0.39 eV for the Zr-containing and 0.77-0.94 eV for the Hf-containing perovskites. These states are centered about 2 Å above the outermost AO atomic layer and dominated by the orbitals of both A-site cations and O from the outermost AO atomic layer, as shown in Figs. 1b,d for SrO-terminated SrHfO$_3$(001). Regardless of the origin, these results indicate that the band gap reduction is indeed a common feature of the cubic perovskite family.

Although LDOS in known to provide a good insight into the spatial distribution of electronic properties, the computed quantity can be affected by the limitations of the projection scheme utilizing spherical approximation of the Wigner-Seitz cells. In particular, the surface charge densities estimated from the layer-resolved LDOS (see Fig. 1b,c) can be affected. To evince that the surface states can accommodate enough charge carriers to alter the surface conductivities considerably, we calculated cumulative charges for the surface states by integrating the surface state densities (see methods, Figs. S4 and S5) over the slab volumes and represented them per unit surface area. The obtained quantity can be interpreted as maximum number of charge carriers that can be accommodated per unit area in the states at the surface of interest. As can be seen in Fig. 1g, the cumulative charges are generally larger for the states at the BO$_2$-terminated surfaces, with the exception of SrHfO$_3$(001). Importantly, for all studied surfaces except BaO-terminated BaTiO$_3$(001), the charges are greater than 5×10$^{-3}$ e/Å$^2$, which is comparable to the electron densities of 2DEG on SrTiO$_3$ surfaces and interfaces. This result indicates that these states can indeed alter the surface conductivities of perovskites considerably and even contribute to the formation of the 2DEG, as it was previously discussed for SrTiO$_3$(001).
To identify the most stable CO$_2$ adsorption conformations, we analyzed all configurations obtained from the screening of over 300 CO$_2$ adsorption positions on SrO- and TiO$_2$-terminated SrTiO$_3$(001) surfaces presented in our recent work.$^{31}$ Most of them were also found after relaxation on the other perovskite surfaces (see Figs. 2a,c and S6), as it could be anticipated from the similar geometries and chemistries of the cubic perovskites. For higher CO$_2$ coverage of 0.50, six and two different coverage modes were analyzed at the AO and BO$_2$ terminations, respectively (see Fig. S7). The most stable adsorption conformations and coverage modes were also investigated accounting for the reduced symmetry due to the surface distortion patterns, as well as by introducing random perturbations to the surface ions. We found that the perturbations can lead to minor stabilization of up to 5 meV/molecule, which signifies thermodynamic stability of the identified conformations and sets an error bar for the CO$_2$ adsorption energy calculations in this work.

The most stable adsorption conformations at Θ=0.25 are nearly identical for all considered materials, with minor differences originated from the surface distortion patterns, as illustrated in Fig. S8. In particular, CO$_2$ interaction with the AO-terminated ABO$_3$(001) results in the formation of highly stable CO$_3$-like complexes, where C and O atoms of the adsorbed molecules are bonded to the surface oxygen (denoted by O$_S$ here) and two separate A-site cations, respectively (see Fig. 2a). From the thermodynamic perspective, molecular CO$_2$ chemisorption on the AO-terminated ABO$_3$(001) is highly favorable, as suggested by their low adsorption energies varying from -2.19 eV for SrZrO$_3$ to -1.79 eV for BaHfO$_3$ (see Fig. 2b). Interestingly, for both Sr- and Ba-containing perovskites, the strongest CO$_2$ adsorption was found for the compounds containing Zr. Considering that optimized geometries of the CO$_3$-like complexes are almost independent of the compound (see Table S5), higher stability of CO$_2$ adsorption here can be associated with lower stresses due to the largest lattice constants of the Zr-containing perovskites (see Table S1). At higher CO$_2$ coverage of 0.50, the chemisorption becomes weaker. Specifically, the molecule-molecule interaction increases the CO$_2$ adsorption energies by 0.24-0.45 eV and even results in stabilization of alternative adsorption modes for BaTiO$_3$ and BaHfO$_3$ (see Fig. S9). These results suggest that the AO-terminated ABO$_3$(001) surfaces can firmly trap atmospheric CO$_2$ by forming a thin layer of CO$_3$-like complexes upon exposure of as-synthesized perovskites to atmospheric air.
CO\textsubscript{2} interaction with the BO\textsubscript{2}-terminated surfaces also leads to the formation of CO\textsubscript{3}-like complexes, where C and O atoms of the adsorbed molecules are bonded to the surface oxygen (O\textsubscript{S}) and B-site atoms, respectively, as shown in Fig. 2c. The C-O\textsubscript{S} bonds and O-C-O angles of the formed CO\textsubscript{3}-like complexes are larger here as compared to those at the AO terminations (see Table S5). The CO\textsubscript{2} adsorption energies for the BO\textsubscript{2}-terminated surfaces at Θ=0.25 are within a range from -1.75 eV for BaHfO\textsubscript{3}(001) to -1.24 eV for SrTiO\textsubscript{3}(001), implying less stable chemisorption compared to that on the AO terminations (see Fig. 2d). The further increase in CO\textsubscript{2} coverage to 0.50 increases adsorption energy by less than 0.1 eV, and therefore, the interaction between the chemisorbed molecules on the BO\textsubscript{2} terminations is weaker.

The CO\textsubscript{2} adsorption on the perovskite surfaces alters their electronic properties by suppressing the surface states. Specifically, energy gaps of the AO-terminated ABO\textsubscript{3}(001) slabs increase considerably to the corresponding bulk values at Θ=0.25 of CO\textsubscript{2} (see Fig. 3a). This change is due to the suppression of the surfaces states at the CBM levels of the clean surfaces, as illustrated in Figs. S11-S26. It should be noted that the energy gaps of some slabs containing CO\textsubscript{2} molecules exceed the corresponding bulk values, which can be attributed to the model geometry constraints and may be eliminated using thicker slabs. These electronic properties persist at Θ=0.50 as well, as shown in Fig. 3a,c. For the BO\textsubscript{2}-terminated surfaces, the band gap energies at Θ=0.25 are 0.31-0.46 eV larger than those for the corresponding clean slabs but are 0.10-0.39 eV smaller than the bulk values, as shown in Fig. 3b. Instead, the surface states at CBM levels are fully suppressed at Θ=0.50 (see Fig. 3d), suggesting a more gradual change of the surface electronic properties upon CO\textsubscript{2} chemisorption on the BO\textsubscript{2}-terminated surfaces. However, more detailed analysis within a wider CO\textsubscript{2} coverage range is needed to predict the concentration-dependent sensing response.

Since sensing response is experimentally defined as a ratio of material resistances in different environments,\textsuperscript{2, 3} a similar first-principles descriptor is needed to quantify the band gap modulation effect. Considering that CO\textsubscript{2} adsorption leads to the complete suppression of the surface states at Θ=0.50, the absolute difference in the band gaps of the bulk and clean slab systems can be employed for such quantification. Although this parameter ignores possible changes in the carrier mobilities, it captures a dominant role played by the band gap changes and accounts for the exponential dependence of the charge carrier concentrations on the energy gap. It should be noted, however, that this approach can only be used to compare sensitivities of the surface layers, whereas electrical conductance of the bulk-like regions is implicitly neglected.
To examine the sensitivity of the proposed parameter to the computational approach, we also computed the band gap reductions for the cubic perovskite surfaces using the hybrid HSE06 functional. As can be seen in Fig. S10, despite the significant difference between the band gap energies of the bulk perovskites computed using PBE and HSE06, the magnitude of the band gap reduction for all investigated BO$_2$-terminated surfaces does not strongly depend on the employed formalism. Specifically, the maximum difference of 0.15 eV only was obtained for HfO$_2$-terminated SrHfO$_3$(001). Furthermore, no drastic change in the surface electronic properties was found for AO-terminated BaTiO$_3$(001) and SrTiO$_3$(001). In contrast, surface states at all other AO-terminated surfaces reduce the band gap energies more drastically when analyzed using the HSE06 approach. Here, the computed differences in the band gap reductions were in 0.34-0.39 eV range for all four representative surfaces. Although the HSE06 approach changes the values of band gap reduction, it does not alter general trends deduced for the surface state, as evident from Fig. S10. Therefore, we can conclude that the PBE results can be employed for the analysis of chemiresistive CO$_2$ sensing response in the considered perovskite systems.

The computed band gap differences for the cubic perovskites are shown in Fig. 3e. The largest band gap modulations of 0.94 and 0.77 eV at AO-terminated SrHfO$_3$(001) and BaHfO$_3$(001) imply their strong potential for chemiresistive CO$_2$ detection. It should be noted, however, that the use of these perovskites can be limited by their relatively large band gap energies, which lead to high electrical resistance, thus making conductivity measurements practically difficult.$^{72}$ At the same time, TiO$_2$-terminated BaTiO$_3$(001) and SrTiO$_3$(001) have the strongest CO$_2$ detection potentials among the considered BO$_2$-terminated surfaces, which is due to the energy gap reductions of 0.82 and 0.78 eV, respectively. It worth mentioning that BaTiO$_3$-containing composites have already been employed as active materials for chemiresistive CO$_2$ detection with great success,$^{7,8,18-21,23-26}$ while SrTiO$_3$ nanostructures are effectively used to sense various reactive gases.$^{73-76}$ Moreover, the use of Ti-containing perovskites is further promoted by their relatively small energy gaps, which can result in lower electrical resistance, and thus simplify electrical circuit needed for the future devices.$^{72}$

Suppression of the surface states represents a new approach to chemiresistive CO$_2$ detection, which may challenge classical ionization mechanism adopted for detection of reactive gases.$^{2,4}$ However, to unleash its full capability, in practice, usage of nanoscale materials with high surface-to-bulk ratios is required due to the strong spatial confinement of the surface states. Apart
from that, when choosing optimal perovskite material for CO₂ detection, low band gap perovskites might be favored as small energy gap generally leads to higher conductivity preferable for the conductivity measurements. It may also be valuable to hypothesize an impact the band gap modulation effect on the optical properties of nanostructured perovskites. Since band gap energy is among the main parameters determining light absorption characteristics of the material, the band gap reduction can also be utilized to develop optical CO₂ sensors. However, such detectors may require compound with the band gap energy in the visible spectral region, whereas more research on the technical aspects of the perovskite-based optical sensors is needed.

Although this work considers the band gap modulation effect from the gas sensing perspective, it can also have considerable impact in other related fields, including catalysis and photocatalysis. From one side, layer of CO₃-like complexes at the most stable (001) surfaces can form a barrier preventing further molecular chemisorption, while from the other side, the formation of such complexes might be a first step in the CO₂ reduction pathways. Moreover, adsorption-induced change in the surface electronic properties may signify a need to reconsider both concentration and localization of photoelectrons as well as overpotentials between the band gap edges of the perovskite-based catalysts and target redox potentials of the catalytic reactions. Finally, since the perovskites are often used as substrate materials for epitaxial growth, the presence of chemisorbed molecules and the corresponding changes in the surface electronic properties may affect the composition and band alignment at the formed interfaces. Because of this, care should be taken to control the concentration of CO₂ species adsorbed on the perovskite substrates during the epitaxial growth.

**Conclusions**

In this work, the effect of band gap modulation by CO₂ adsorption on (001) surfaces of six different cubic perovskites with the general formula of ABO₃ (A = Ba, Sr and B = Ti, Zr, Hf) was assessed using first-principles methods. The results reveal an appearance of surface states at most clean surfaces. For the BO₂-terminated ABO₃(001), the states emerge above the bulk VBM levels and are confined to the outermost BO₂ atomic layer, reducing the energy gaps of the slab systems by 0.41-0.82 eV. For the AO-terminated ABO₃(001), the surface states appear below the bulk CBM level and are localized either at the subsurface BO₂ layer or about 2 Å above the outermost AO atomic layer. The first scenario applies to TiO₂-terminated SrTiO₃(001) and results in the band
gap reduction of 0.24 eV, while the second is observed for the Zr- and Hf-containing compounds and leads to the narrowing of the band gaps by 0.27-0.39 and 0.77-0.94 eV, respectively. Moreover, the surface electronics of the studied perovskites can change upon the CO$_2$ chemisorption, which is accompanied by the formation of stable CO$_3$-like complexes. For most AO-terminated surfaces, $\Theta=0.25$ coverage is sufficient to suppress the surface states completely, whereas for the BO$_2$-terminated surface, the same effect is only achieved at the higher $\Theta=0.50$ coverage. Based on these results, we can conclude that TiO$_2$-terminated BaTiO$_3$(001) and SrTiO$_3$(001) are the most prospective CO$_2$ sensing materials among all studied systems due to the high computed band gap reductions of 0.82 and 0.78 eV, respectively, and relatively low band gap energies of their bulk forms. The AO-terminated SrHfO$_3$(001) and BaHfO$_3$(001) are also promising candidates for chemiresistive CO$_2$ detection due to even larger band gap modulations of 0.94 and 0.77 eV, respectively. However, the application of these surfaces can be limited by practical difficulties associated with measuring low conductivities inherent to the compounds with large band gaps.

**Electronic supplementary information (ESI) available**

Additional information on the surface geometry, electronic properties, and optimized slab structures of the perovskite systems are provided.

**Conflicts of interest**

There are no conflicts to declare.

**Acknowledgments**

The authors acknowledge the support from the SUTD-ZJU (ZJURP1200101), MOE Tier2 (T2 MOE1201-Singapore), and Research Council of Norway (contracts: 221469, 250346, 251131). Most of this work was performed on the Abel cluster, owned by the University of Oslo and the Norwegian Metacenter for Computational Science (NOTUR), and operated by the Department for Research Computing at USIT, the University of Oslo IT-department. The authors also acknowledge PRACE for awarding access to resource MareNostrum based in Spain at BSC-CNS.
References

1. T. Seiyama, A. Kato, K. Fujiishi and M. Nagatani, Analytical Chemistry, 1962, 34, 1502-1503.
2. H.-J. Kim and J.-H. Lee, Sensors and Actuators B: Chemical, 2014, 192, 607-627.
3. K. Wetchakun, T. Samerjai, N. Tamaekong, C. Liewhiran, C. Siriwong, V. Kruefu, A. Wisitsoraat, A. Tuantranont and S. Phanichphant, Sensors and Actuators B: Chemical, 2011, 160, 580-591.
4. G. Korotcenkov and B. Cho, Sensors and Actuators B: Chemical, 2017, 244, 182-210.
5. H. Jane and P. T. Ralph, Measurement Science and Technology, 2013, 24, 012004.
6. S. N. Habisreutinger, L. Schmidt-Mende and J. K. Stolarczyk, Angewandte Chemie International Edition, 2013, 52, 7372-7408.
7. A. Haesler and J.-U. Meyer, Sensors and Actuators B: Chemical, 1996, 34, 388-395.
8. M.-S. Lee and J.-U. Meyer, Sensors and Actuators B: Chemical, 2000, 68, 293-299.
9. L. Cavanagh, P. Smith and R. Binions, Journal of the Electrochemical Society, 2012, 159, J67-J71.
10. C. R. Michel, A. H. Martínez, F. Huerta-Villalpando and J. P. Morán-Lázaro, Journal of Alloys and Compounds, 2009, 484, 605-611.
11. E. Delgado and C. R. Michel, Materials Letters, 2006, 60, 1613-1616.
12. L. Li, H. Qin, C. Shi, L. Zhang, Y. Chen and J. Hu, RSC Advances, 2015, 5, 103073-103081.
13. K. Fan, H. Qin, L. Wang, L. Ju and J. Hu, Sensors and Actuators B: Chemical, 2013, 177, 265-269.
14. P. Zhang, H. Qin, H. Zhang, W. Lu and J. Hu, Journal of Rare Earths, 2017, 35, 602-609.
15. X. Wang, Y. Chen, H. Qin, L. Li, C. Shi, L. Liu and J. Hu, Physical Chemistry Chemical Physics, 2015, 17, 13733-13742.
16. X. Wang, H. Qin, L. Sun and J. Hu, Sensors and Actuators B: Chemical, 2013, 188, 965-971.
17. Y. Chen, H. Qin, C. Shi, L. Li and J. Hu, RSC Advances, 2015, 5, 54710-54716.
18. P. Keller, H. Ferkel, K. Zweiacker, J. Naser, J.-U. Meyer and W. Riehemann, Sensors and Actuators B: Chemical, 1999, 57, 39-46.
19. T. Ishihara, M. Higuchi, T. Takagi, M. Ito, H. Nishiguchi and Y. Takita, Journal of Materials Chemistry, 1998, 8, 2037-2042.
20. B. Liao, Q. Wei, K. Wang and Y. Liu, Sensors and Actuators B: Chemical, 2001, 80, 208-214.
21. S. Joshi, S. J. Ippolito, S. Periasamy, Y. M. Sabri and M. V. Sunkara, ACS Applied Materials & Interfaces, 2017, 9, 27014-27026.
22. J. Herrán, G. G. Mandayo and E. Castaño, Sensors and Actuators B: Chemical, 2007, 127, 370-375.
23. J. Herrán, G. G. Mandayo, N. Pérez, E. Castano, A. Prim, E. Pellicer, T. Andreu, F. Peiro, A. Cornet and J. Morante, Sensors and Actuators B: Chemical, 2008, 133, 315-320.
24. J. Herrán, G. G. Mandayo and E. Castano, Thin Solid Films, 2009, 517, 6192-6197.
25. J. Herrán, G. G. Mandayo, I. Ayerdi and E. Castano, Sensors and Actuators B: Chemical, 2008, 129, 386-390.
26. J. Herrán, O. Fernández-González, I. Castro-Hurtado, T. Romero, G. G. Mandayo and E. Castano, Sensors and Actuators B: Chemical, 2010, 149, 368-372.
27. J. Baniecki, M. Ishii, K. Kurihara, K. Yamanaka, T. Yano, K. Shinozaki, T. Imada and Y. Kobayashi, Journal of Applied Physics, 2009, 106, 4109.
28. J. Baniecki, M. Ishii, K. Kurihara, K. Yamanaka, T. Yano, K. Shinozaki, T. Imada, K. Nozaki and N. Kin, Physical Review B, 2008, 78, 195415.
29. Y. Shen, W. Wang, X. Wang, Z. Zhou and W. Fei, Applied Surface Science, 2014, 308, 269-274.
30. W. Wang, Y. Shen, X. Wang, Z. Zhou and W. Fei, Applied Surface Science, 2014, 298, 102-108.
31. K. V. Sopiha, O. I. Malyi, C. Persson and P. Wu, Physical Chemistry Chemical Physics, 2017, 19, 16629-16637.
32. N. P. Guisinger, T. S. Santos, J. R. Guest, T.-Y. Chien, A. Bhattacharya, J. W. Freeland and M. Bode, ACS Nano, 2009, 3, 4132-4136.
33. N. Plumb, M. Salluzzo, E. Razzoli, M. Månsson, M. Falub, J. Krempasky, C. Matt, J. Chang, M. Schulte and J. Braun, Physical Review Letters, 2014, 113, 086801.
34. P. King, R. He, T. Eknapakul, P. Buaphet, S.-K. Mo, Y. Kaneko, S. Harashima, Y. Hikita, M. Bahramy and C. Bell, Physical Review Letters, 2012, 108, 117602.
35. P. Delugas, V. Fiorentini, A. Mattoni and A. Filippetti, Physical Review B, 2015, 91, 115315.
36. G. Kresse and J. Hafner, Physical Review B, 1993, 47, 558.
37. G. Kresse and J. Furthmüller, Computational Materials Science, 1996, 6, 15-50.
38. G. Kresse and J. Furthmüller, Physical Review B, 1996, 54, 11169.
39. J. P. Perdew, K. Burke and M. Ernzerhof, Physical Review Letters, 1996, 77, 3865.
40. G. Kresse and D. Joubert, Physical Review B, 1999, 59, 1758.
41. P. E. Blöchl, Physical Review B, 1994, 50, 17953.
42. H. J. Monkhorst and J. D. Pack, Physical Review B, 1976, 13, 5188.
43. M. Chan and G. Ceder, Physical Review Letters, 2010, 105, 196403.
44. A. V. Krukau, O. A. Vydrov, A. F. Izmaylov and G. E. Scuseria, Journal of Chemical Physics, 2006, 125, 224106.
45. K. Momma and F. Izumi, Journal of Applied Crystallography, 2011, 44, 1272-1276.
46. S. P. Ong, W. D. Richards, A. Jain, G. Hautier, M. Kocher, S. Cholia, D. Gunter, V. L. Chevrier, K. A. Persson and G. Ceder, Computational Materials Science, 2013, 68, 314-319.
47. P. Goudochnikov and A. J. Bell, Journal of Physics: Condensed Matter, 2007, 19, 176201.
48. R. Eglitis and D. Vanderbilt, Physical Review B, 2008, 78, 155420.
49. R. Eglitis and M. Rohlfing, Journal of Physics: Condensed Matter, 2010, 22, 415901.
50. F. Sánchez, C. Ocal and J. Fontcuberta, Chemical Society Reviews, 2014, 43, 2272-2285.
51. E. H. Morales and D. A. Bonnell, Surface Science, 2013, 609, 62-66.
52. A. M. Kolpak, D. Li, R. Shao, A. M. Rappe and D. A. Bonnell, *Physical Review Letters*, 2008, **101**, 036102.
53. J. M. P. Martínez, E. H. Morales, W. A. Saidi, D. A. Bonnell and A. M. Rappe, *Physical Review Letters*, 2012, **109**, 256802.
54. R. Shimizu, K. Iwaya, T. Ohsawa, S. Shiraki, T. Hasegawa, T. Hashizume and T. Hitosugi, *Applied Physics Letters*, 2012, **100**, 263106.
55. K. Johnston, M. R. Castell, A. T. Paxton and M. W. Finnis, *Physical Review B*, 2004, **70**, 085415.
56. F. Silly, D. T. Newell and M. R. Castell, *Surface Science*, 2006, **600**, 219-223.
57. N. Iles, F. Finocchi and K. D. Khodja, *Journal of Physics: Condensed Matter*, 2010, **22**, 305001.
58. L. Bengtsson, *Physical Review B*, 1999, **59**, 12301.
59. R. D. Shannon, *Acta Crystallographica Section A: Crystal Physics, Diffraction, Theoretical and General Crystallography*, 1976, **32**, 751-767.
60. L. Pauling, *The nature of the chemical bond and the structure of molecules and crystals: an introduction to modern structural chemistry*, Cornell University Press, 1960.
61. J. G. Speight, *Lange's handbook of chemistry*, McGraw-Hill New York, 2005.
62. V. M. Goldschmidt, *Naturwissenschaften*, 1926, **14**, 477-485.
63. C. Li, K. C. K. Soh and P. Wu, *Journal of Alloys and Compounds*, 2004, **372**, 40-48.
64. R. Eglitis and A. Popov, *Journal of Saudi Chemical Society*, 2018, **22**, 459-468.
65. S. Piskunov, E. Kotomin, E. Heifets, J. Maier, R. Eglitis and G. Borstel, *Surface Science*, 2005, **575**, 75-88.
66. O. I. Malyi, K. V. Sopiha, I. Radchenko, P. Wu and C. Persson, *Physical Chemistry Chemical Physics*, 2018, **20**, 2075-2083.
67. Q. Xu, K. Sopiha, M. Sobhan, F. Anariba, K. P. Ong, J. W. Zheng and P. Wu, *Applied Physics Letters*, 2016, **108**, 011602.
68. S. Maintz, V. L. Deringer, A. L. Tchougréeff and R. Dronskowski, *Journal of Computational Chemistry*, 2013, **34**, 2557-2567.
69. W. Meevasana, P. D. C. King, R. H. He, S. K. Mo, M. Hashimoto, A. Tamai, P. Songsiriiritthigul, F. Bumberger and Z. X. Shen, *Nature Materials*, 2011, **10**, 114-118.
70. A. F. Santander-Syro, O. Copie, T. Kondo, F. Fortuna, S. Pailhes, R. Weht, X. G. Qiu, F. Bertran, A. Nicolaou, A. Taleb-Ibrahimi, P. Le Fevre, G. Herranz, M. Bibes, N. Reyren, Y. Apertet, P. Lecoeur, A. Barthelemy and M. J. Rozenberg, *Nature*, 2011, **469**, 189-193.
71. N. Reyren, S. Thiel, A. Caviglia, L. F. Kourkoutis, G. Hammerl, C. Richter, C. Schneider, T. Kopp, A.-S. Rüetschi and D. Jaccard, *Science*, 2007, **317**, 1196-1199.
72. G. Korotcenkov, *Materials Science and Engineering: B*, 2007, **139**, 1-23.
73. T. Hara and T. Ishiguro, *Sensors and Actuators B: Chemical*, 2009, **136**, 489-493.
74. Y. Hu, O. Tan, J. Pan and X. Yao, *Journal of Physical Chemistry B*, 2004, **108**, 11214-11218.
75. A. M. Schultz, T. D. Brown and P. R. Ohodnicki Jr, *Journal of Physical Chemistry C*, 2015, **119**, 6211-6220.
76. K. Sahner, R. Moos, M. Matam, J. J. Tunney and M. Post, Sensors and Actuators B: Chemical, 2005, 108, 102-112.
Figures and Captions
Figure 1. Electronic properties of (001) cubic perovskite surfaces. (a) Computed band gap energies of the bulk and slab ABO$_3$ systems. Typical layer-resolved local density of states (LDOS).
illustrated for clean (b) SrO- and (c) HfO$_2$-terminated SrHfO$_3$(001) surfaces (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 the layer-resolved LDOS neglecting the population densities below 0.3 1/eV/layer). More details on electronic properties of the other considered surfaces are given in Figs. S11-S26. In-plane averaged surface state densities for (d) SrO- and (e) HfO$_2$-terminated SrHfO$_3$(001), as well as (f) SrO-terminated SrTiO$_3$(001) surfaces (see Figs. S4 and S5 for the surface state localization at the other perovskite surfaces). (g) Cumulative charges for surface states at the ABO$_3$(001).
Figure 2. Most stable CO$_2$ adsorption conformations on (a) BaO- and (c) TiO$_2$-terminated BaTiO$_3$(001) surfaces corresponding to $\Theta=0.25$. More details on CO$_2$ adsorption conformations for the other perovskite surfaces, metastable configurations, and higher ($\Theta=0.50$) coverage can be found in Figs. S6-S9. Computed CO$_2$ adsorption energies for the (b) AO- and (d) BO$_2$-terminated ABO$_3$(001) surfaces. The adsorption energies are tabulated in Tables S3 and S4.
Figure 3. Computed band gap energies of the (a) AO- and (b) BO₂-terminated ABO₃(001) surfaces containing zero (Θ=0.00), one (Θ=0.25), and two (Θ=0.50) adsorbed CO₂ molecules. Band gap energies of the corresponding bulk systems are given for comparison. Typical layer-resolved local density of states (LDOS) for (c) SrO- and (d) HfO₂-terminated SrHfO₃(001) containing Θ=0.50 CO₂ coverage (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 the layer-resolved LDOS neglecting the population densities below 0.3 1/eV/layer). (e) Computed difference in the band gap energies of the bulk and clean slab perovskite systems. More details on electronic properties of the other perovskite systems containing chemisorbed CO₂ are given in Figs. S11-S26.
Supplementary information:

Suppression of Surfaces States at Cubic Perovskite (001) Surfaces by CO$_2$ Adsorption

*Kostiantyn V. Sopiha', Oleksandr I. Malyi$^{2*}$, Clas Persson$^2$, Ping Wu$^{1*}$

1 – Entropic Interface Group, Engineering Product Development, Singapore University of Technology and Design, 8 Somapah Road, 487372 Singapore, Singapore

2 – Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo, P. O. Box 1048 Blindern, NO-0316 Oslo, Norway

E-mails: oleksandrmalyi@gmail.com (O.I.M), wuping@sutd.edu.sg (W.P)
List of tables

**Table S1.** Consolidated properties of the cubic perovskites ................................................................. 25
**Table S2.** Consolidated properties of the clean ABO$_3$(001) surfaces .................................................. 26
**Table S3.** Consolidated properties of the ABO$_3$(001) surfaces at $\Theta=0.25$ CO$_2$ coverage .......... 27
**Table S4.** Consolidated properties of the ABO$_3$(001) surfaces at $\Theta=0.50$ CO$_2$ coverage .......... 28
**Table S5.** Geometries of the CO$_3$-like complexes formed upon CO$_2$ chemisorption on the ABO$_3$(001) surfaces of cubic perovskites at $\Theta=0.25$ ................................................................. 29

List of figures

**Figure S1.** Projected density of states (DOS) for all considered cubic perovskite materials ....... 30
**Figure S2.** Most stable surface distortion for all considered cubic perovskite surfaces .............. 31
**Figure S3.** Stabilization energies for different perovskite ABO$_3$(001) surfaces ......................... 32
**Figure S4.** Localization of the surface states at the Sr-containing ABO$_3$(001) ......................... 33
**Figure S5.** Localization of the surface states at the Ba-containing ABO$_3$(001) ......................... 34
**Figure S6.** Metastable CO$_2$ adsorption conformations observed on AO-terminated BaTiO$_3$(001) surface. All systems correspond to $\Theta=0.25$ CO$_2$ coverage ................................................................. 35
**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 $\Theta=0.50$ CO$_2$ coverage ........ 36
**Figure S8.** Surface relaxations upon CO$_2$ adsorption at $\Theta=0.25$ coverage .............................. 37
**Figure S9.** Surface relaxations upon CO$_2$ adsorption at $\Theta=0.50$ coverage .............................. 38
**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 .................................................................................................................. 39
**Figure S11.** Layer-resolved local density of states (LDOS) for SrO-terminated SrTiO$_3$(001) .... 40
**Figure S12.** Layer-resolved local density of states (LDOS) for SrO-terminated SrZrO$_3$(001) ....... 41
**Figure S13.** Layer-resolved local density of states (LDOS) for SrO-terminated SrHfO$_3$(001) .... 42
**Figure S14.** Layer-resolved local density of states (LDOS) for BaO-terminated BaTiO$_3$(001) ... 43
**Figure S15.** Layer-resolved local density of states (LDOS) for BaO-terminated BaZrO$_3$(001) .. 44
**Figure S16.** Layer-resolved local density of states (LDOS) for BaO-terminated BaHfO$_3$(001) .. 45
**Figure S17.** Layer-resolved local density of states (LDOS) for TiO$_2$-terminated SrTiO$_3$(001) .. 46
Figure S18. Layer-resolved local density of states (LDOS) for ZrO2-terminated SrZrO3(001)...
Figure S19. Layer-resolved local density of states (LDOS) for HfO2-terminated SrHfO3(001)...
Figure S20. Layer-resolved local density of states (LDOS) for TiO2-terminated BaTiO3(001)...
Figure S21. Layer-resolved local density of states (LDOS) for ZrO2-terminated BaZrO3(001)...
Figure S22. Layer-resolved local density of states (LDOS) for HfO2-terminated BaHfO3(001)...
Figure S23. Projected density of states (DOS) for two surface layers of the Sr-containing AO-terminated ABO3(001)........................................................................................................52
Figure S24. Projected density of states (DOS) for two surface layers of the Ba-containing AO-terminated ABO3(001)........................................................................................................53
Figure S25. Projected density of states (DOS) for two surface layers of the Sr-containing BO2-terminated ABO3(001)........................................................................................................54
Figure S26. Projected density of states (DOS) for two surface layers of the Ba-containing BO2-terminated ABO3(001)........................................................................................................55

List of structures

Structure 1. SrO-terminated SrTiO3 slab at Θ=0.00 CO2 coverage..............................................56
Structure 2. SrO-terminated SrTiO3 slab at Θ=0.25 CO2 coverage..............................................60
Structure 3. SrO-terminated SrTiO3 slab at Θ=0.50 CO2 coverage..............................................64
Structure 4. SrO-terminated SrZrO3 slab at Θ=0.00 CO2 coverage..............................................68
Structure 5. SrO-terminated SrZrO3 slab at Θ=0.25 CO2 coverage..............................................72
Structure 6. SrO-terminated SrZrO3 slab at Θ=0.50 CO2 coverage..............................................76
Structure 7. SrO-terminated SrHfO3 slab at Θ=0.00 CO2 coverage.............................................80
Structure 8. SrO-terminated SrHfO3 slab at Θ=0.25 CO2 coverage.............................................84
Structure 9. SrO-terminated SrHfO3 slab at Θ=0.50 CO2 coverage.............................................88
Structure 10. BaO-terminated BaTiO3 slab at Θ=0.00 CO2 coverage..........................................92
Structure 11. BaO-terminated BaTiO3 slab at Θ=0.25 CO2 coverage..........................................96
Structure 12. BaO-terminated BaTiO3 slab at Θ=0.50 CO2 coverage.........................................100
Structure 13. BaO-terminated BaZrO3 slab at Θ=0.00 CO2 coverage........................................104
Structure 14. BaO-terminated BaZrO3 slab at Θ=0.25 CO2 coverage........................................108
Structure 15. BaO-terminated BaZrO3 slab at Θ=0.50 CO2 coverage........................................112
Structure 16. BaO-terminated BaHfO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ................................................. 116
Structure 17. BaO-terminated BaHfO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage .................................................. 120
Structure 18. BaO-terminated BaHfO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage .................................................. 124
Structure 19. TiO\(_2\)-terminated SrTiO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 128
Structure 20. TiO\(_2\)-terminated SrTiO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 132
Structure 21. TiO\(_2\)-terminated SrTiO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 136
Structure 22. ZrO\(_2\)-terminated SrZrO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 140
Structure 23. ZrO\(_2\)-terminated SrZrO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 144
Structure 24. ZrO\(_2\)-terminated SrZrO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 148
Structure 25. HfO\(_2\)-terminated SrHfO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 152
Structure 26. HfO\(_2\)-terminated SrHfO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 156
Structure 27. HfO\(_2\)-terminated SrHfO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 160
Structure 28. TiO\(_2\)-terminated BaTiO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 164
Structure 29. TiO\(_2\)-terminated BaTiO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 168
Structure 30. TiO\(_2\)-terminated BaTiO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 172
Structure 31. ZrO\(_2\)-terminated BaZrO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 176
Structure 32. ZrO\(_2\)-terminated BaZrO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 180
Structure 33. ZrO\(_2\)-terminated BaZrO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 184
Structure 34. HfO\(_2\)-terminated BaHfO\(_3\) slab at \(\Theta=0.00\) CO\(_2\) coverage ........................................... 188
Structure 35. HfO\(_2\)-terminated BaHfO\(_3\) slab at \(\Theta=0.25\) CO\(_2\) coverage ........................................... 192
Structure 36. HfO\(_2\)-terminated BaHfO\(_3\) slab at \(\Theta=0.50\) CO\(_2\) coverage ........................................... 196
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.$^{59}$

| 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 ABO₃(001) surfaces at Θ=0.50 CO₂ coverage.

| Compound   | Termination | PBE band gap (eV) | CO₂ adsorption energy (eV) |
|------------|-------------|-------------------|----------------------------|
| SrTiO₃     | SrO         | 1.85              | -1.47                      |
|            | TiO₂        | 1.81              | -1.20                      |
| SrZrO₃     | SrO         | 3.28              | -1.95                      |
|            | ZrO₂        | 3.26              | -1.60                      |
| SrHfO₃     | SrO         | 3.82              | -1.81                      |
|            | HfO₂        | 3.80              | -1.59                      |
| BaTiO₃     | BaO         | 1.75              | -1.38                      |
|            | TiO₂        | 1.73              | -1.43                      |
| BaZrO₃     | BaO         | 3.05              | -1.60                      |
|            | ZrO₂        | 3.00              | -1.62                      |
| BaHfO₃     | BaO         | 3.54              | -1.46                      |
|            | HfO₂        | 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$_5$ 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.
|          | SrTiO₃ | SrZrO₃ | SrHfO₃ |
|----------|--------|--------|--------|
| AO-terminated (001) | ![Image](image1.png) | ![Image](image2.png) | ![Image](image3.png) |
| BO₂-terminated (001) | ![Image](image4.png) | ![Image](image5.png) | ![Image](image6.png) |
|          | BaTiO₃ | BaZrO₃ | BaHfO₃ |
| AO-terminated (001) | ![Image](image7.png) | ![Image](image8.png) | ![Image](image9.png) |
| BO₂-terminated (001) | ![Image](image10.png) | ![Image](image11.png) | ![Image](image12.png) |

- Green: Sr
- Orange: Ba
- Blue: Ti
- Yellow: Zr
- Light Grey: Hf
- Red: O

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 $\Theta$=0.25 CO$_2$ coverage. $\Delta E_{ads}$ 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 $\Theta$=0.50 CO$_2$ coverage.
|                | SrTiO$_3$          | SrZrO$_3$          | SrHfO$_3$          |
|----------------|--------------------|--------------------|--------------------|
| AO-terminated (001) | ![SrTiO$_3$] | ![SrZrO$_3$] | ![SrHfO$_3$] |
| BO$_2$-terminated (001) | ![SrTiO$_3$] | ![SrZrO$_3$] | ![SrHfO$_3$] |
| AO-terminated (001) | ![BaTiO$_3$] | ![BaZrO$_3$] | ![BaHfO$_3$] |
| BO$_2$-terminated (001) | ![BaTiO$_3$] | ![BaZrO$_3$] | ![BaHfO$_3$] |

Figure S8. Surface relaxations of all considered perovskite surfaces upon CO$_2$ adsorption at Θ=0.25 coverage.
Figure S9. Surface relaxations of all considered perovskite surfaces upon CO$_2$ adsorption at $\Theta=0.50$ 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 5d²6s², zirconium 4d²5s², and titanium 3d²4s² 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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).
**BaO-terminated BaTiO$_3$(001)**

\( \Theta = 0.00 \) \hspace{1cm} \( \Theta = 0.25 \) \hspace{1cm} \( \Theta = 0.50 \)

Figure S14. Layer-resolved local density of states (LDOS) for BaO-terminated BaTiO$_3$(001) at \( \Theta=0.00 \) (clean surface), \( \Theta=0.25 \), and \( \Theta=0.50 \) 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 from 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 from 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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).
HfO$_2$-terminated SrHfO$_3$(001)

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\textsubscript{2}-terminated BaTiO\textsubscript{3}(001) at $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ CO\textsubscript{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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 $\text{ABO}_3(001)$ at $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 $\text{ABO}_3(001)$ at $\Theta=0.00$ (clean surface), $\Theta=0.25$, and $\Theta=0.50$ 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 BO₂-terminated ABO₃(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO₂ 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 BO2-terminated ABO3(001) at Θ=0.00 (clean surface), Θ=0.25, and Θ=0.50 CO2 coverages. The numbers represent band gap energies of the slab systems.
Structure 1. SrO-terminated SrTiO$_3$ slab at $\Theta=0.00$ 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 0.590881 |
| 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 0.000000 0.499998 |
| Sr    | 0.499857 0.499857 0.499998 |
| Sr    | 0.000804 0.001697 0.768100 |
| Sr    | 0.000804 0.501647 0.768107 |
| Sr    | 0.500756 0.001696 0.768107 |
| Sr    | 0.500756 0.501646 0.768113 |
| Sr    | 0.001474 0.002035 0.680663 |
| Sr    | 0.001473 0.501981 0.680665 |
| Sr    | 0.501420 0.002033 0.680665 |
| Sr    | 0.501419 0.501979 0.680666 |
| Sr    | 0.000000 0.000000 0.409119 |
| Sr    | 0.000000 0.499857 0.409119 |
| Sr    | 0.499857 0.000000 0.409119 |
| Sr    | 0.499857 0.499857 0.409119 |
| Sr    | 0.000804 0.001697 0.231900 |
| Sr    | 0.000804 0.501647 0.231893 |
| Sr    | 0.500756 0.001696 0.231893 |
| Sr    | 0.500756 0.501646 0.231887 |
| Sr    | 0.001474 0.002035 0.319337 |
| Sr    | 0.001473 0.501981 0.319335 |
| Sr    | 0.501420 0.002033 0.319335 |
| Sr    | 0.501419 0.501979 0.319334 |
| Ti    | 0.249929 0.249929 0.545440 |
| Ti    | 0.249929 0.749786 0.545440 |
| Ti    | 0.749786 0.249929 0.545440 |
| Ti    | 0.749786 0.749786 0.545440 |
| Ti    | 0.250992 0.251786 0.728941 |
Ti  0.250993  0.751729  0.728946
Ti  0.750932  0.251788  0.728946
Ti  0.750933  0.751731  0.728946
Ti  0.252199  0.252808  0.636662
Ti  0.252204  0.752757  0.636664
Ti  0.752146  0.252813  0.636664
Ti  0.752151  0.752762  0.636665
Ti  0.250992  0.251786  0.271059
Ti  0.250993  0.751729  0.271054
Ti  0.750932  0.251788  0.271054
Ti  0.750933  0.751731  0.271049
Ti  0.252199  0.252808  0.363338
Ti  0.252204  0.752757  0.363336
Ti  0.752146  0.252813  0.363336
Ti  0.752151  0.752762  0.363335
O  0.249929  0.000000  0.545440
O  0.249929  0.499857  0.545440
O  0.749786  0.000000  0.545440
O  0.749786  0.499857  0.545440
O  0.249929  0.249929  0.590881
O  0.249929  0.749786  0.590881
O  0.749786  0.249929  0.590881
O  0.749786  0.749786  0.590881
O  0.000000  0.249929  0.545440
O  0.000000  0.749786  0.545440
O  0.499857  0.249929  0.545440
O  0.499857  0.749786  0.545440
O  0.249929  0.249929  0.499998
O  0.249929  0.749786  0.499998
O  0.749786  0.249929  0.499998
O  0.749786  0.749786  0.499998
O  0.249555  0.249173  0.773230
O  0.249555  0.749072  0.773229
O  0.749457  0.249172  0.773229
O  0.749456  0.749072  0.773228
O  0.499703  0.249754  0.727918
O  0.499702  0.749664  0.727919
O  0.999706  0.249755  0.727919
O  0.999706  0.749665  0.727920
O  0.249294  0.249080  0.681918
O  0.249294  0.748986  0.681919
O  0.749201  0.249079  0.681919
|   |   |   |   |
|---|---|---|---|
| O | 0.248894 | 0.998711 | 0.363516 |
| O | 0.748799 | 0.498698 | 0.363515 |
| O | 0.748800 | 0.998709 | 0.363515 |
Structure 2. SrO-terminated SrTiO$_3$ slab at $\Theta$=0.25 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 0.013161 0.489044 0.226694 |
| Sr 0.993750 0.000464 0.228305 |
| Sr 0.501160 0.506908 0.228361 |
| Sr 0.489349 0.011608 0.230341 |
| Sr 0.002269 0.008371 0.318484 |
| Sr 0.492689 0.007673 0.318496 |
| Sr 0.491811 0.498027 0.318555 |
| Sr 0.005809 0.494379 0.318587 |
| Sr 0.500000 0.000000 0.409118 |
| Sr 0.500000 0.499857 0.409118 |
| Sr 0.000143 0.000000 0.409118 |
| Sr 0.000143 0.499857 0.409118 |
| Sr 0.500000 0.000000 0.499998 |
| Sr 0.500000 0.499857 0.499998 |
| Sr 0.000143 0.000000 0.499998 |
| Sr 0.000143 0.499857 0.499998 |
| Sr 0.500000 0.000000 0.590882 |
| Sr 0.500000 0.499857 0.590882 |
| Sr 0.000143 0.000000 0.590882 |
| Sr 0.000143 0.499857 0.590882 |
| Sr 0.005809 0.494379 0.681413 |
| Sr 0.491811 0.498027 0.681445 |
| Sr 0.492689 0.007673 0.681504 |
| Sr 0.002269 0.008371 0.681516 |
| Sr 0.489349 0.011608 0.769659 |
| Sr 0.501160 0.506908 0.771639 |
| Sr 0.993750 0.000464 0.771695 |
| Sr 0.013161 0.489044 0.773306 |
| Ti 0.749972 0.254607 0.269181 |
| Ti 0.246156 0.750961 0.269206 |
| Ti 0.247512 0.253407 0.270446 |
| Ti 0.748356 0.752031 0.276150 |
| Ti 0.747169 0.255935 0.362536 |
Ti  0.244262  0.753075  0.362541
Ti  0.248255  0.251970  0.363540
Ti  0.747846  0.752394  0.365028
Ti  0.250071  0.249929  0.454560
Ti  0.750214  0.249929  0.454560
Ti  0.750214  0.749786  0.454560
Ti  0.250071  0.749786  0.545440
Ti  0.750214  0.749786  0.545440
Ti  0.747846  0.752394  0.634972
Ti  0.748356  0.752031  0.723850
C  0.793181  0.707221  0.197485
C  0.793181  0.707221  0.802515
O  0.942999  0.760424  0.190324
O  0.247512  0.253407  0.729554
C  0.793181  0.707221  0.197485
C  0.793181  0.707221  0.802515
O  0.942999  0.760424  0.190324
O  0.247512  0.253407  0.729554
O  0.246156  0.750961  0.730794
O  0.749972  0.254607  0.730819
O  0.248255  0.251970  0.636456
O  0.244262  0.753075  0.637459
O  0.747169  0.255935  0.637464
O  0.749972  0.254607  0.730819
O  0.248255  0.251970  0.636456
O  0.244262  0.753075  0.637459
O  0.747169  0.255935  0.637464
O  0.749972  0.254607  0.730819
O  0.750214  0.249929  0.545440
O  0.750214  0.749786  0.545440
O  0.747846  0.752394  0.634972
O  0.248255  0.251970  0.636456
O  0.244262  0.753075  0.637459
O  0.747169  0.255935  0.637464
O  0.749972  0.254607  0.730819
O  0.748356  0.752031  0.723850
O  0.247085  0.252757  0.226540
O  0.753884  0.220707  0.227456
O  0.278820  0.745087  0.227456
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  0.246586  0.499480  0.272958
O  0.506299  0.745280  0.274438
O  0.501403  0.998497  0.274497
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
O  0.253041  0.498423  0.363345
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
O  0.500000  0.749786  0.454560
O  0.500000  0.249929  0.454560
O  0.000143  0.749786  0.454560
O  0.000143  0.249929  0.454560
O  0.250071  0.249929  0.499998
O  0.250071  0.749786  0.499998
O  0.750214  0.249929  0.499998
O  0.750214  0.749786  0.499998
O  0.250071  0.000000  0.545440
O  0.250071  0.499857  0.545440
O  0.750214  0.000000  0.545440
O  0.750214  0.499857  0.545440
O  0.750214  0.000000  0.545440
O  0.750214  0.499857  0.545440
O  0.750590  0.499653  0.635275
O  0.000266  0.747465  0.635277
O  0.251502  0.998497  0.636121
O  0.501403  0.246625  0.636129
O  0.001430  0.248447  0.636653
O  0.253041  0.498423  0.636655
O  0.504094  0.748936  0.638140
O  0.752617  0.995804  0.638152
O  0.253192  0.246645  0.681642
O  0.237722  0.751355  0.681834
O  0.748569  0.262440  0.681848
O  0.769586  0.730304  0.682612
O  0.750642  0.993635  0.725503
O  0.506299  0.745280  0.725562
O  0.246586  0.499480  0.727042
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 $\Theta$=0.50 CO$_2$ coverage

```plaintext
_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  0.506888  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  0.499857  0.499857  0.409119
  Sr  0.499857  0.000000  0.409119
  Sr  0.01787  0.995832  0.317842
  Sr  0.00915  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  0.500478  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
```
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
Ti  0.749786  0.749786  0.545440
Ti  0.749786  0.749786  0.454560
Ti  0.749786  0.249929  0.454560
Ti  0.249929  0.749786  0.454560
Ti  0.756156  0.744251  0.364899
Ti  0.256278  0.246458  0.364864
Ti  0.752350  0.244568  0.362024
Ti  0.252121  0.742821  0.362011
Ti  0.248482  0.246580  0.275086
Ti  0.749344  0.749499  0.274989
Ti  0.749600  0.250648  0.268255
Ti  0.250132  0.744449  0.268118
C  0.797421  0.713648  0.803373
C  0.296717  0.286027  0.803274
C  0.296717  0.286027  0.196726
C  0.797421  0.713648  0.196627
O  0.209282  0.209090  0.780115
O  0.709609  0.788564  0.779966
O  0.277534  0.769762  0.772455
O  0.776741  0.229830  0.772406
O  0.995806  0.743747  0.733145
O  0.495941  0.247593  0.732659
O  0.253484  0.495785  0.732032
O  0.744948  0.503493  0.731804
O  0.245468  0.003291  0.726005
O  0.753824  0.996356  0.725937
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
O 0.253484 0.495785 0.267968
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 $\Theta=0.00$ 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  0.500000
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  0.505364  0.495239  0.680163
Sr  0.465410  0.489142  0.766726
Sr  0.500000  0.000000  0.590909
Sr  0.493708  0.003240  0.319831
Sr  0.489626  0.964777  0.233279
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  0.319781
Sr  0.965637  0.989622  0.233255
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
```
| Element | X Value | Y Value | Z Value |
|---------|---------|---------|---------|
| 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 |
| 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       | 0.50728 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       | 0.50090 0.199881 0.731772 |
| O       | 0.500000 0.750000 0.545455 |
| O       | 0.500368 0.807686 0.634130 |
| O       | 0.000198 0.807686 0.634130 |
| 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       | 0.73638 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 |
|   |   |   |
|---|---|---|
| 0.232933 | 0.302252 | 0.770668 |
| 0.750000 | 0.500000 | 0.545455 |
| 0.807622 | 0.500332 | 0.633891 |
| 0.701082 | 0.499503 | 0.732011 |
| 0.750000 | 0.000000 | 0.545455 |
| 0.699898 | 0.000749 | 0.637977 |
| 0.802974 | 0.001018 | 0.721287 |
| 0.250000 | 0.500000 | 0.545455 |
| 0.199969 | 0.500769 | 0.638032 |
| 0.303015 | 0.500975 | 0.721270 |
| 0.250000 | 0.000000 | 0.545455 |
| 0.307587 | 0.000380 | 0.633857 |
| 0.200919 | 0.999478 | 0.731983 |
| 0.500000 | 0.750000 | 0.454545 |
| 0.500728 | 0.700015 | 0.362184 |
| 0.501773 | 0.801961 | 0.278540 |
| 0.500000 | 0.250000 | 0.454545 |
| 0.500338 | 0.307767 | 0.365930 |
| 0.500090 | 0.199881 | 0.268228 |
| 0.000000 | 0.750000 | 0.454545 |
| 0.000368 | 0.807686 | 0.365870 |
| 0.000198 | 0.699620 | 0.268456 |
| 0.000000 | 0.250000 | 0.454545 |
| 0.000715 | 0.200069 | 0.362103 |
| 0.001672 | 0.301793 | 0.278627 |
| 0.750000 | 0.750000 | 0.409091 |
| 0.774332 | 0.723556 | 0.318650 |
| 0.733638 | 0.802240 | 0.229317 |
| 0.750000 | 0.250000 | 0.409091 |
| 0.726136 | 0.277089 | 0.318623 |
| 0.802410 | 0.232305 | 0.229336 |
| 0.250000 | 0.750000 | 0.409091 |
| 0.227111 | 0.777511 | 0.318634 |
| 0.302182 | 0.732166 | 0.229337 |
| 0.250000 | 0.250000 | 0.409091 |
| 0.275022 | 0.223442 | 0.318641 |
| 0.232933 | 0.302252 | 0.229332 |
| 0.750000 | 0.500000 | 0.454545 |
| 0.807622 | 0.500332 | 0.366109 |
| 0.701082 | 0.499503 | 0.267989 |
| 0.750000 | 0.000000 | 0.454545 |
| 0.699898 | 0.000749 | 0.366109 |
| 0.802974 | 0.001018 | 0.278713 |
| 0.250000 | 0.500000 | 0.454545 |
| 0.199969 | 0.500769 | 0.361968 |
| 0.303015 | 0.500975 | 0.278730 |
Structure 5. SrO-terminated SrZrO$_3$ slab at $\Theta$=0.25 CO$_2$ coverage

```
_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 0.500000 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
```
Zr  0.247782  0.247756  0.636226
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
C  0.808719  0.719018  0.792852
C  0.808719  0.719018  0.207148
O  0.274401  0.501145  0.716502
O  0.694103  0.505054  0.729886
O  0.219101  0.001328  0.735689
O  0.800655  0.998446  0.721737
O  0.221425  0.213268  0.681202
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
O  0.290582  0.293512  0.770900
O  0.710706  0.798128  0.774784
O  0.776388  0.573088  0.799038
O  0.937418  0.786937  0.801324
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  0.200338  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 | 0.750000 | 0.750000 | 0.590909 |
| O | 0.702280 | 0.998840 | 0.639239 |
| O | 0.250000 | 0.250000 | 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 | 0.500000 | 0.250000 | 0.545455 |
| O | 0.750000 | 0.000000 | 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 | 0.503166 | 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 |
Structure 6. SrO-terminated SrZrO$_3$ slab at $\Theta=0.50$ 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'

Atom site information:

| Symbol | Fractional coordinates |
|--------|------------------------|
| 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 |
| Element | X  | Y  | Z   |
|---------|----|----|-----|
| 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 | 0.545455 |
| 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 |
| O       | 0.902687 | 0.814131 | 0.193441 |
| O       | 0.751835 | 0.735991 | 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 |
0.785766 0.996618 0.719638
0.201635 0.004252 0.721576
0.000037 0.298510 0.721871
0.494194 0.199306 0.729807
0.290670 0.497802 0.732750
0.707429 0.503405 0.733524
0.995202 0.720926 0.737349
0.319991 0.797525 0.769263
0.791914 0.209875 0.769336
0.702888 0.803044 0.773630
0.204210 0.208603 0.774687
0.424792 0.270518 0.800429
0.215509 0.436338 0.800912
0.751835 0.591832 0.802339
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 0.500909
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
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 $\Theta=0.25$ CO$_2$ coverage

```plaintext
_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  0.317321
Sr  0.500000  0.500000  0.409091
Sr  0.000771  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 | 0.774676 | 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  0.970930  0.462635  0.227991
Sr  0.993480  0.992132  0.231467
Sr  0.497591  0.504559  0.316649
Sr  0.50267  0.010658  0.317448
Sr  0.00134  0.989868  0.319877
Sr  0.00130  0.494139  0.320701
Sr  0.50000  0.50000  0.409091
Sr  0.00000  0.00000  0.409091
Sr  0.00000  0.50000  0.409091
Sr  0.00000  0.00000  0.500000
Sr  0.00000  0.50000  0.500000
Sr  0.50000  0.50000  0.500000
Sr  0.50000  0.50000  0.590909
Sr  0.50000  0.00000  0.590909
Sr  0.50000  0.50000  0.590909
Sr  0.00000  0.00000  0.590909
Sr  0.00130  0.494139  0.679299
Sr  0.00134  0.989868  0.680123
Sr  0.500267  0.010658  0.768533
Sr  0.497591  0.504559  0.833351
Sr  0.993480  0.992132  0.773458
Sr  0.487469  0.548858  0.776633
Hf  0.249707  0.751817  0.270847
Hf  0.745476  0.248590  0.275194
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 0.49936 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 0.750000 0.750000 0.500000
O 0.750000 0.250000 0.500000
O 0.250000 0.250000 0.500000
O 0.250000 0.750000 0.500000
O 0.000000 0.750000 0.545455
O 0.000000 0.250000 0.545455
O 0.500000 0.250000 0.545455
O 0.500000 0.750000 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 0.49936 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 $\Theta$=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 0.270825
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  0.750000  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

| Atom | _atom_site_type_symbol | _atom_site_fract_x | _atom_site_fract_y | _atom_site_fract_z |
|------|-------------------------|--------------------|--------------------|--------------------|
| Ba   | Ba                      | 0.000000           | 0.500000           | 0.500000           |
| Ba   | Ba                      | 0.000000           | 0.500000           | 0.590909           |
| Ba   | Ba                      | 0.006546           | 0.500191           | 0.682518           |
| Ba   | Ba                      | 0.013002           | 0.493897           | 0.775977           |
| Ba   | Ba                      | 0.000000           | 0.000000           | 0.500000           |
| Ba   | Ba                      | 0.000000           | 0.000000           | 0.590909           |
| Ba   | Ba                      | 0.006029           | 0.006035           | 0.682421           |
| Ba   | Ba                      | 0.998907           | 0.996853           | 0.774923           |
| Ba   | Ba                      | 0.500000           | 0.500000           | 0.500000           |
| Ba   | Ba                      | 0.500000           | 0.500000           | 0.590909           |
| Ba   | Ba                      | 0.499357           | 0.499371           | 0.682573           |
| Ba   | Ba                      | 0.506804           | 0.503125           | 0.776005           |
| Ba   | Ba                      | 0.500000           | 0.000000           | 0.500000           |
| Ba   | Ba                      | 0.500000           | 0.000000           | 0.590909           |
| Ba   | Ba                      | 0.499654           | 0.006977           | 0.682398           |
| Ba   | Ba                      | 0.494286           | 0.011085           | 0.773640           |
| Ba   | Ba                      | 0.494286           | 0.011085           | 0.226360           |
| Ba   | Ba                      | 0.499654           | 0.006977           | 0.317602           |
| Ba   | Ba                      | 0.500000           | 0.000000           | 0.409091           |
| Ba   | Ba                      | 0.506804           | 0.503125           | 0.223995           |
| Ba   | Ba                      | 0.499357           | 0.499371           | 0.317427           |
| Ba   | Ba                      | 0.500000           | 0.500000           | 0.409091           |
| Ba   | Ba                      | 0.998907           | 0.996853           | 0.225077           |
| Ba   | Ba                      | 0.006029           | 0.006035           | 0.317579           |
| Ba   | Ba                      | 0.000000           | 0.000000           | 0.409091           |
| Ba   | Ba                      | 0.013002           | 0.493897           | 0.224022           |
| Ba   | Ba                      | 0.006546           | 0.500191           | 0.317482           |
| Ba   | Ba                      | 0.000000           | 0.500000           | 0.409091           |
| Ti   | Ti                      | 0.250000           | 0.250000           | 0.545455           |
| Ti   | Ti                      | 0.259705           | 0.259747           | 0.636998           |
| Ti   | Ti                      | 0.257313           | 0.260069           | 0.730189           |
| Ti   | Ti                      | 0.250000           | 0.750000           | 0.545455           |
| Ti   | Ti                      | 0.261156           | 0.759576           | 0.637789           |
| Element | X | Y | Z |
|---------|---|---|---|
| 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 | 0.365579 |
| 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 | 0.795818 | 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 | 0.746069 | 0.989593 | 0.637042 |
| O | 0.745052 | 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  | 0.745538  | 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 $\Theta=0.50$ CO$_2$ coverage

```plaintext
_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  0.000000  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  0.634985
Ti  0.750000  0.250000  0.454545
Ti  0.250000  0.250000  0.454545
Ti  0.250000  0.250000  0.454545
Ti  0.750000  0.250000  0.454545
Ti  0.250000  0.750000  0.454545
Ti  0.750000  0.750000  0.454545
Ti  0.741591  0.741199  0.365039
Ti  0.241697  0.241213  0.365014
Ti  0.739550  0.239457  0.361699
Ti  0.756053  0.742087  0.273901
Ti  0.244257  0.241982  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  0.009303  0.729484
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
| X  | Y  | Z   |
|----|----|-----|
| 0.254331 | 0.010709 | 0.636859 |
| 0.750000 | 0.750000 | 0.590909 |
| 0.250000 | 0.750000 | 0.590909 |
| 0.750000 | 0.250000 | 0.590909 |
| 0.250000 | 0.250000 | 0.590909 |
| 0.750000 | 0.000000 | 0.545455 |
| 0.750000 | 0.500000 | 0.545455 |
| 0.250000 | 0.000000 | 0.545455 |
| 0.000000 | 0.750000 | 0.545455 |
| 0.500000 | 0.250000 | 0.545455 |
| 0.500000 | 0.750000 | 0.545455 |
| 0.750000 | 0.750000 | 0.500000 |
| 0.750000 | 0.250000 | 0.500000 |
| 0.250000 | 0.750000 | 0.500000 |
| 0.250000 | 0.250000 | 0.500000 |
| 0.500000 | 0.250000 | 0.454545 |
| 0.500000 | 0.750000 | 0.454545 |
| 0.000000 | 0.750000 | 0.454545 |
| 0.000000 | 0.250000 | 0.454545 |
| 0.250000 | 0.000000 | 0.454545 |
| 0.750000 | 0.500000 | 0.454545 |
| 0.750000 | 0.000000 | 0.454545 |
| 0.250000 | 0.500000 | 0.454545 |
| 0.250000 | 0.250000 | 0.409091 |
| 0.750000 | 0.250000 | 0.409091 |
| 0.250000 | 0.750000 | 0.409091 |
| 0.750000 | 0.750000 | 0.409091 |
| 0.254331 | 0.010709 | 0.363141 |
| 0.754300 | 0.510723 | 0.363124 |
| 0.010729 | 0.254174 | 0.363105 |
| 0.510528 | 0.754225 | 0.363094 |
| 0.004869 | 0.754108 | 0.363034 |
| 0.505158 | 0.254148 | 0.362990 |
| 0.254090 | 0.505218 | 0.362987 |
| 0.754030 | 0.005288 | 0.362979 |
| 0.252315 | 0.754155 | 0.319105 |
| 0.753398 | 0.254122 | 0.319069 |
| 0.252214 | 0.252565 | 0.315680 |
| 0.751512 | 0.752575 | 0.315670 |
| 0.751015 | 0.509404 | 0.270560 |
| 0.251845 | 0.009303 | 0.270516 |
| 0.750754 | 0.007809 | 0.270359 |
| 0.251935 | 0.507941 | 0.270352 |
| 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 $\Theta=0.00$ 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  0.000000  0.000000  0.409091
Ba  0.000000  0.000000  0.318956
Ba  0.000000  0.000000  0.230018
Ba  0.000000  0.500000  0.409091
Ba  0.000000  0.500000  0.318956
Ba  0.000000  0.500000  0.230018
Ba  0.999886  0.000275  0.681038
Ba  0.999101  0.012349  0.769988
Ba  0.000000  0.500000  0.409091
Ba  0.000000  0.500000  0.318956
Ba  0.000000  0.500000  0.230018
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
```
| Element | X | Y | Z |
|---------|---|---|---|
| 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 | 0.636562 |
| Zr      | 0.247803 | 0.751627 | 0.728508 |
| Zr      | 0.750000 | 0.250000 | 0.545455 |
| 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 |
| 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       | 0.755528 | 0.755425 | 0.681948 |
| O       | 0.744237 | 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 0.000000 0.750000 0.454545
O 0.000067 0.738122 0.364074
O 0.999436 0.778285 0.270489
Structure 14. BaO-terminated BaZrO₃ slab at Θ=0.25 CO₂ coverage

|    | _cell_length_a  | _cell_length_b  | _cell_length_c  | _cell_angle_alpha | _cell_angle_beta | _cell_angle_gamma | _symmetry_space_group_name_H-M  |
|----|----------------|----------------|-----------------|-------------------|-----------------|-------------------|--------------------------------|
|    | 8.51149400     | 8.51149400     | 46.81321300     | 90.00000000       | 90.00000000     | 90.00000000      | 'P 1'                          |

|    | loop_          | _atom_site_type_symbol | _atom_site_fract_x | _atom_site_fract_y | _atom_site_fract_z |
|----|----------------|------------------------|--------------------|--------------------|--------------------|
|    | _atom_site_type_symbol | Ba                    | 0.024347 0.496789 0.226304 |
|    | _atom_site_fract_x    | Ba                    | 0.002389 0.011395 0.227529 |
|    | _atom_site_fract_y    | Ba                    | 0.498800 0.504631 0.228366 |
|    | _atom_site_fract_z    | Ba                    | 0.497355 0.016792 0.229395 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.003275 0.002844 0.318301 |
|    | _atom_site_fract_x    | Ba                    | 0.497418 0.003868 0.318374 |
|    | _atom_site_fract_y    | Ba                    | 0.004184 0.496092 0.318547 |
|    | _atom_site_fract_z    | Ba                    | 0.496478 0.497134 0.318662 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.500000 0.000000 0.409091 |
|    | _atom_site_fract_x    | Ba                    | 0.500000 0.500000 0.409091 |
|    | _atom_site_fract_y    | Ba                    | 0.000000 0.500000 0.409091 |
|    | _atom_site_fract_z    | Ba                    | 0.000000 0.000000 0.409091 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.500000 0.000000 0.500000 |
|    | _atom_site_fract_x    | Ba                    | 0.500000 0.500000 0.500000 |
|    | _atom_site_fract_y    | Ba                    | 0.000000 0.000000 0.500000 |
|    | _atom_site_fract_z    | Ba                    | 0.000000 0.000000 0.500000 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.500000 0.000000 0.590909 |
|    | _atom_site_fract_x    | Ba                    | 0.500000 0.500000 0.590909 |
|    | _atom_site_fract_y    | Ba                    | 0.000000 0.000000 0.590909 |
|    | _atom_site_fract_z    | Ba                    | 0.000000 0.000000 0.590909 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.496478 0.497134 0.681338 |
|    | _atom_site_fract_x    | Ba                    | 0.004184 0.496092 0.681453 |
|    | _atom_site_fract_y    | Ba                    | 0.497418 0.003868 0.681626 |
|    | _atom_site_fract_z    | Ba                    | 0.003275 0.002844 0.681699 |
|    | loop_          | _atom_site_type_symbol | Ba                    | 0.497355 0.016792 0.770605 |
|    | _atom_site_fract_x    | Ba                    | 0.496478 0.497134 0.771634 |
|    | _atom_site_fract_y    | Ba                    | 0.000000 0.001395 0.772471 |
|    | _atom_site_fract_z    | Ba                    | 0.024347 0.496789 0.773696 |
|    | loop_          | _atom_site_type_symbol | Zr                    | 0.753209 0.252464 0.270649 |
|    | _atom_site_fract_x    | Zr                    | 0.251671 0.750630 0.270799 |
|    | _atom_site_fract_y    | Zr                    | 0.250492 0.252478 0.271762 |
|    | _atom_site_fract_z    | Zr                    | 0.751062 0.751393 0.274398 |
|    | loop_          | _atom_site_type_symbol | Zr                    | 0.749732 0.250661 0.363107 |

|    | _atom_site_fract_x    | Zr                    | 0.750000 0.000000 0.363107 |
|    | _atom_site_fract_y    | Zr                    | 0.500000 0.500000 0.363107 |
|    | _atom_site_fract_z    | Zr                    | 0.000000 0.000000 0.363107 |

|    | loop_          | _atom_site_type_symbol | Zr                    | 0.750000 0.000000 0.363107 |
|    | _atom_site_fract_x    | Zr                    | 0.500000 0.500000 0.363107 |
|    | _atom_site_fract_y    | Zr                    | 0.000000 0.000000 0.363107 |
|    | _atom_site_fract_z    | Zr                    | 0.000000 0.000000 0.363107 |

|    | loop_          | _atom_site_type_symbol | Zr                    | 0.750000 0.000000 0.363107 |
|    | _atom_site_fract_x    | Zr                    | 0.500000 0.500000 0.363107 |
|    | _atom_site_fract_y    | Zr                    | 0.000000 0.000000 0.363107 |
|    | _atom_site_fract_z    | Zr                    | 0.000000 0.000000 0.363107 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Zr   | 0.249426 | 0.750511 | 0.363153 |
| Zr   | 0.250642 | 0.249028 | 0.636847 |
| 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   | 0.751180 | 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  | 0.272134 | 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 $\Theta$=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    | 0.000000              | 0.000000          | 0.590909          |
| Ba    | 0.500000              | 0.000000          | 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 0.545455
Zr 0.750000 0.250000 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  0.250000  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  0.000000  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  0.750000  0.000000  0.635080
O  0.001018  0.260167  0.637706
O  0.266428  0.500000  0.636030
O  0.238039  0.743588  0.681659
O  0.737164  0.255893  0.681708
O  0.500000  0.250000  0.635101
O  0.239314  0.001018  0.637615
O  0.999392  0.739271  0.635774
O  0.500947  0.500844  0.636303
O  0.760946  0.999286  0.636828
O  0.239314  0.001018  0.637615
O  0.500947  0.760771  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
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 |
| 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 BaHfO₃ slab at Θ=0.00 CO₂ 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' |

| _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         |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| 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 |
| 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       | 0.250846 | 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 |
| X1   | Y1   | Z1   |
|------|------|------|
| 0.256755 | 0.255654 | 0.772733 |
| 0.500000 | 0.750000 | 0.545455 |
| 0.500374 | 0.751280 | 0.636292 |
| 0.500788 | 0.750428 | 0.728721 |
| 0.500000 | 0.250000 | 0.545455 |
| 0.500364 | 0.248968 | 0.636660 |
| 0.500738 | 0.250424 | 0.727396 |
| 0.000000 | 0.750000 | 0.545455 |
| 0.000377 | 0.748979 | 0.636722 |
| 0.000787 | 0.750434 | 0.727266 |
| 0.000000 | 0.250000 | 0.545455 |
| 0.000361 | 0.251274 | 0.636338 |
| 0.000736 | 0.250376 | 0.728571 |
| 0.750000 | 0.000000 | 0.454545 |
| 0.751624 | 0.000156 | 0.363330 |
| 0.750685 | 0.000463 | 0.272555 |
| 0.750000 | 0.500000 | 0.454545 |
| 0.749311 | 0.500150 | 0.363651 |
| 0.750770 | 0.500459 | 0.271448 |
| 0.250000 | 0.000000 | 0.454545 |
| 0.249240 | 0.000134 | 0.363663 |
| 0.250846 | 0.000407 | 0.271462 |
| 0.250000 | 0.500000 | 0.454545 |
| 0.251571 | 0.500130 | 0.363330 |
| 0.250851 | 0.500404 | 0.272566 |
| 0.750000 | 0.750000 | 0.409091 |
| 0.748259 | 0.748573 | 0.318054 |
| 0.757663 | 0.755764 | 0.227268 |
| 0.750000 | 0.250000 | 0.409091 |
| 0.752286 | 0.252086 | 0.318056 |
| 0.744723 | 0.245256 | 0.227259 |
| 0.250000 | 0.750000 | 0.409091 |
| 0.252889 | 0.752025 | 0.318057 |
| 0.244123 | 0.745075 | 0.227272 |
| 0.250000 | 0.250000 | 0.409091 |
| 0.248738 | 0.248493 | 0.318061 |
| 0.256755 | 0.255654 | 0.227267 |
| 0.500000 | 0.750000 | 0.454545 |
| 0.500374 | 0.751280 | 0.363708 |
| 0.500788 | 0.750428 | 0.271279 |
| 0.500000 | 0.250000 | 0.454545 |
| 0.500364 | 0.248968 | 0.363340 |
| 0.500738 | 0.250424 | 0.272604 |
| 0.000000 | 0.750000 | 0.454545 |
| 0.000377 | 0.748979 | 0.363278 |
| 0.000787 | 0.750434 | 0.272734 |
|   | 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 $\Theta=0.25$ CO$_2$ coverage

```plaintext
_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 0.500000 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 0.772434  
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
```
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Hf      | 0.749743 | 0.250226 | 0.363217 |
| Hf      | 0.250752 | 0.249373 | 0.363709 |
| Hf      | 0.751119 | 0.748904 | 0.364004 |
| Hf      | 0.250000 | 0.750000 | 0.454545 |
| Hf      | 0.250000 | 0.250000 | 0.454545 |
| Hf      | 0.750000 | 0.250000 | 0.454545 |
| Hf      | 0.750000 | 0.750000 | 0.454545 |
| Hf      | 0.250000 | 0.750000 | 0.545455 |
| Hf      | 0.250000 | 0.250000 | 0.545455 |
| Hf      | 0.750000 | 0.750000 | 0.545455 |
| Hf      | 0.250000 | 0.250000 | 0.635996 |
| 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  | 0.748936  | 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 0.500254 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\textsubscript{3} slab at Θ=0.50 CO\textsubscript{2} coverage

\begin{verbatim}
_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  0.002708  0.502635  0.682066
 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  0.250094  0.274492
 Hf  0.250920  0.750094  0.362932
\end{verbatim}
| X   | Y   | Z   |
|-----|-----|-----|
| 0.750621 | 0.250025 | 0.363311 |
| 0.749167 | 0.749800 | 0.364146 |
| 0.249618 | 0.249773 | 0.364170 |
| 0.250000 | 0.250000 | 0.454545 |
| 0.750000 | 0.250000 | 0.454545 |
| 0.749167 | 0.749800 | 0.635854 |
| 0.249067 | 0.749617 | 0.727816 |
| 0.749664 | 0.748889 | 0.198216 |
| 0.749664 | 0.748889 | 0.801784 |
| 0.386629 | 0.244820 | 0.185128 |
| 0.737047 | 0.883719 | 0.186057 |
| 0.252639 | 0.248644 | 0.197728 |
| 0.749664 | 0.748889 | 0.198216 |
| 0.750621 | 0.250025 | 0.363311 |
| 0.249618 | 0.249773 | 0.364170 |
| 0.750000 | 0.250000 | 0.454545 |
| 0.250920 | 0.750094 | 0.637068 |
| 0.250876 | 0.250001 | 0.725508 |
| 0.750762 | 0.749793 | 0.725537 |
| 0.751680 | 0.249693 | 0.727816 |
| 0.249067 | 0.749617 | 0.731025 |
| 0.750621 | 0.250025 | 0.363311 |
| 0.250920 | 0.750094 | 0.637068 |
| 0.751680 | 0.249693 | 0.727816 |
| 0.249067 | 0.749617 | 0.731025 |

| C   | O   |
|-----|-----|
| 0.749664 | 0.748889 |
| 0.749664 | 0.748889 |
| 0.252639 | 0.248644 |
| 0.386629 | 0.244820 |
| 0.737047 | 0.883719 |
| 0.113396 | 0.246371 |
| 0.741180 | 0.610662 |
| 0.220468 | 0.745740 |
| 0.259067 | 0.256281 |
| 0.776265 | 0.752704 |
| 0.740359 | 0.247163 |
| 0.502807 | 0.749673 |
| 0.249996 | 0.002526 |
| 0.002147 | 0.249675 |
| 0.749742 | 0.501349 |
| 0.250253 | 0.497516 |
| 0.749786 | 0.998134 |
| 0.498828 | 0.249946 |
| 0.997315 | 0.749954 |
| 0.257551 | 0.751342 |
| 0.739806 | 0.748761 |
| 0.245986 | 0.248215 |
| 0.753944 | 0.250688 |
| 0.999319 | 0.750506 |
| 0.499438 | 0.250536 |
| 0.249399 | 0.499361 |
| 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 |
| 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  | 0.000000 | 0.000000 | 0.454545 |
| O  | 0.750000 | 0.500000 | 0.454545 |
| O  | 0.250000 | 0.500000 | 0.454545 |
| O  | 0.250000 | 0.750000 | 0.454545 |
| O  | 0.750000 | 0.750000 | 0.454545 |
| O  | 0.750000 | 0.250000 | 0.500000 |
| O  | 0.750000 | 0.750000 | 0.500000 |
| O  | 0.250000 | 0.000000 | 0.545455 |
| O  | 0.250000 | 0.750000 | 0.545455 |
| O  | 0.000000 | 0.250000 | 0.545455 |
| O  | 0.000000 | 0.750000 | 0.545455 |
| O  | 0.250000 | 0.500000 | 0.545455 |
| O  | 0.750000 | 0.500000 | 0.545455 |
| O  | 0.000000 | 0.250000 | 0.590909 |
| O  | 0.250000 | 0.250000 | 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 0.727476  
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 $\Theta=0.00$ CO$_2$ coverage

```plaintext
_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  0.269406
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
```
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

.Cell parameters:
- _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 information:
- _symmetry_space_group_name_H-M_ 'P 1'

Atom coordinates:
- _atom_site_type_symbol_ Sr
  - Sr 0.496769 0.494562 0.270389
  - 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 0.997384 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
- _atom_site_type_symbol_ Ti
  - Ti 0.770631 0.734773 0.226846
  - Ti 0.23012 0.735810 0.226971
  - Ti 0.740760 0.237827 0.230364
  - Ti 0.499929 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
Ti 0.749786 0.749786 0.499998
Ti 0.249929 0.249929 0.499998
Ti 0.749786 0.749786 0.590882
Ti 0.249929 0.749786 0.590882
Ti 0.749786 0.749786 0.590882
Ti 0.244146 0.241982 0.680883
Ti 0.742476 0.242261 0.680897
Ti 0.243816 0.742195 0.682542
Ti 0.743860 0.742153 0.682542
Ti 0.241353 0.237416 0.769592
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
O 0.499857 0.249929 0.409118
O 0.249929 0.249929 0.454560
O 0.249929 0.749786 0.454560
O 0.749786 0.249929 0.454560
O 0.749786 0.749786 0.454560
O 0.249929 0.000000 0.499998
O 0.249929 0.499857 0.499998
O 0.749786 0.000000 0.499998
O 0.000000 0.249929 0.499998
O 0.499857 0.249929 0.499998
O 0.000000 0.749786 0.499998
O 0.499857 0.749786 0.499998
O 0.249929 0.249929 0.545440
O 0.249929 0.749786 0.545440
O 0.749786 0.249929 0.545440
O 0.749786 0.749786 0.545440
O 0.249929 0.000000 0.590882
O 0.749786 0.000000 0.590882
O 0.249929 0.499857 0.590882
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
O 0.752572 0.250555 0.636311
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. TiO2-terminated SrTiO3 slab at Θ=0.50 CO2 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  0.499472  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  0.000000  0.499857  0.454560
Sr  0.499857  0.000000  0.454560
Sr  0.499857  0.499857  0.545440
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  0.636432
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
| X  | Y  | Z  |
|----|----|----|
| 0.249929 0.249929 0.409119 |
| 0.749786 0.249929 0.499998 |
| 0.249929 0.749786 0.499998 |
| 0.749786 0.749786 0.499998 |
| 0.249929 0.749786 0.590881 |
| 0.249929 0.249929 0.681913 |
| 0.247523 0.742418 0.681913 |
| 0.249477 0.242426 0.681924 |
| 0.749494 0.742435 0.681924 |
| 0.228509 0.733981 0.772348 |
| 0.728519 0.233989 0.772351 |
| 0.271307 0.233972 0.772355 |
| 0.771271 0.733977 0.772361 |
| 0.499907 0.749667 0.197732 |
| 0.999909 0.249710 0.197738 |
| 0.999909 0.249710 0.802262 |
| 0.499907 0.749667 0.802268 |
| 0.645980 0.752595 0.185582 |
| 0.145990 0.252651 0.185585 |
| 0.499908 0.281952 0.225314 |
| 0.999906 0.781930 0.225322 |
| 0.499918 0.740873 0.229225 |
| 0.999920 0.240885 0.229231 |
| 0.270712 0.009066 0.230356 |
| 0.770705 0.509068 0.230358 |
| 0.229077 0.509067 0.230378 |
| 0.729073 0.009053 0.230380 |
| 0.245246 0.755678 0.272509 |
| 0.745229 0.255682 0.272510 |
| 0.254995 0.255617 0.272512 |
| 0.754963 0.755607 0.272517 |
| 0.000409 0.256472 0.317453 |
| 0.500421 0.756470 0.317458 |
| 0.254022 0.503416 0.318274 |
| 0.754024 0.003403 0.318281 |
| 0.246631 0.003365 0.318293 |
| 0.746633 0.503381 0.318296 |
| 0.500345 0.249707 0.318625 |
| 0.500345 0.249707 0.318625 |
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 0.009067 0.769622
O 0.770705 0.009068 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 $\Theta=0.00$ CO$_2$ coverage

```plaintext
_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
```
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  0.000000  0.500000  0.545455
Sr  0.000000  0.000000  0.545455
Sr  0.000148  0.519149  0.636751
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  0.757671  0.250457  0.768620
O  0.249447  0.251011  0.680771
O  0.242445  0.250563  0.768614
O  0.757671  0.250457  0.768620
O  0.764292  0.751207  0.769681
O  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  | 0.702530 | 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  0.000000  0.500000  0.454545
Sr  0.500000  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  0.000293  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 0.681287
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 0.363441
O 0.222169 0.747609 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  | 0.750465 | 0.749326 | 0.318824 |
| Hf  | 0.750000 | 0.250000 | 0.409091 |
| Hf  | 0.746780 | 0.249323 | 0.318776 |
| Hf  | 0.250000 | 0.000000 | 0.500000 |
| Hf  | 0.250000 | 0.500000 | 0.500000 |
| Hf  | 0.750000 | 0.000000 | 0.500000 |
| Hf  | 0.750000 | 0.500000 | 0.500000 |
| O   | 0.000000 | 0.250000 | 0.500000 |
| O   | 0.998905 | 0.291550 | 0.686281 |
| O   | 0.998901 | 0.707901 | 0.675973 |
| O   | 0.998497 | 0.753065 | 0.776386 |
| O   | 0.000000 | 0.250000 | 0.500000 |
| O   | 0.998905 | 0.291550 | 0.686281 |
| O   | 0.998527 | 0.247771 | 0.766120 |
| O   | 0.750000 | 0.250000 | 0.590909 |
| O   | 0.728232 | 0.756774 | 0.636499 |
| O   | 0.785254 | 0.743174 | 0.726697 |
| O   | 0.750000 | 0.250000 | 0.590909 |
| O   | 0.770597 | 0.251625 | 0.590909 |
| 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 0.636510
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 $\Theta$=0.25 CO$_2$ coverage

|   | cell_length_a | cell_length_b | cell_length_c | cell_angle_alpha | cell_angle_beta | cell_angle_gamma | symmetry_space_group_name_H-M |
|---|--------------|---------------|--------------|-----------------|----------------|-----------------|-------------------------------|
|   | 8.28657000   | 8.28657000    | 45.57613800  | 90.00000000     | 90.00000000    | 90.00000000     | '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 0.250909 0.769112 |
| Hf | 0.750000 0.750000 0.590909 |
| Hf | 0.746461 0.751028 0.681885 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| 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 | 0.770625 |
| Hf      | 0.750000 | 0.250000 | 0.409091 |
| Hf      | 0.753995 | 0.250090 | 0.319068 |
| Hf      | 0.750000 | 0.750000 | 0.409091 |
| Hf      | 0.746461 | 0.751028 | 0.318114 |
| 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 |
|   |   |   |
|---|---|---|
| 0.287077 | 0.749716 | 0.272799 |
| 0.750000 | 0.500000 | 0.409091 |
| 0.704972 | 0.499764 | 0.318866 |
| 0.752848 | 0.501118 | 0.231742 |
| 0.750000 | 0.000000 | 0.409091 |
| 0.794528 | 0.000072 | 0.318217 |
| 0.747057 | 0.999268 | 0.232323 |
| 0.250000 | 0.500000 | 0.409091 |
| 0.293503 | 0.499767 | 0.318757 |
| 0.245089 | 0.501121 | 0.231833 |
| 0.250000 | 0.000000 | 0.409091 |
| 0.203963 | 0.000080 | 0.318327 |
| 0.251002 | 0.999274 | 0.232251 |
Structure 27. HfO$_2$-terminated SrHfO$_3$ slab at $\Theta=0.50$ CO$_2$ coverage

| 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 |
| Element | x Coord  | y Coord  | z Coord  |
|---------|----------|----------|----------|
| Hf      | 0.250000 | 0.750000 | 0.409091 |
| Hf      | 0.750000 | 0.250000 | 0.409091 |
| Hf      | 0.750000 | 0.750000 | 0.500000 |
| 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      | 0.750000 | 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 |
163

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 $\Theta=0.00$ CO$_2$ coverage

_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
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| 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      | 0.736971     | 0.762219     | 0.770329     |
| Ti      | 0.250000     | 0.250000     | 0.409091     |
| Ti      | 0.236917     | 0.239160     | 0.318540     |
| Ti      | 0.236942     | 0.262189     | 0.229670     |
| 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 |
|   | 0.012359 | 0.743217 | 0.226865 |
|---|----------|----------|----------|
|   | 0.500000 | 0.250000 | 0.409091 |
|   | 0.507455 | 0.254349 | 0.318154 |
|   | 0.512379 | 0.243234 | 0.226865 |
|   | 0.500000 | 0.750000 | 0.409091 |
|   | 0.507459 | 0.754367 | 0.318154 |
|   | 0.512346 | 0.743233 | 0.226868 |
Structure 29. TiO$_2$-terminated BaTiO$_3$ slab at $\Theta=0.25$ CO$_2$ coverage

_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 0.997656 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

_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'

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
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| 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      | 0.238194   | 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   |
| X   | Y   | Z   |
|-----|-----|-----|
| 0.25323 | 0.492158 | 0.681733 |
| 0.75000 | 0.750000 | 0.545455 |
| 0.750616 | 0.748715 | 0.636241 |
| 0.75000 | 0.250000 | 0.545455 |
| 0.751092 | 0.248601 | 0.636294 |
| 0.750000 | 0.750000 | 0.500000 |
| 0.500000 | 0.750000 | 0.590909 |
| 0.507712 | 0.746432 | 0.682439 |
| 0.500000 | 0.250000 | 0.500000 |
| 0.500000 | 0.250000 | 0.590909 |
| 0.507005 | 0.246649 | 0.681630 |
| 0.500000 | 0.750000 | 0.500000 |
| 0.007657 | 0.746734 | 0.681820 |
| 0.000000 | 0.250000 | 0.500000 |
| 0.007939 | 0.246977 | 0.681652 |
| 0.759070 | 0.987592 | 0.227483 |
| 0.753099 | 0.486061 | 0.228479 |
| 0.247239 | 0.986697 | 0.227597 |
| 0.251750 | 0.486413 | 0.228446 |
| 0.754424 | 0.748247 | 0.271909 |
| 0.751028 | 0.245607 | 0.273032 |
| 0.247805 | 0.747439 | 0.271877 |
| 0.253035 | 0.245806 | 0.272974 |
| 0.501544 | 0.743750 | 0.228489 |
| 0.511372 | 0.241136 | 0.227301 |
| 0.000917 | 0.741893 | 0.225217 |
| 0.010568 | 0.243604 | 0.227753 |
| 0.357728 | 0.738631 | 0.186096 |
| 0.644044 | 0.739571 | 0.186004 |
| 0.750000 | 0.000000 | 0.409091 |
| 0.752598 | 0.991945 | 0.318185 |
| 0.750000 | 0.500000 | 0.409091 |
| 0.752562 | 0.491931 | 0.318226 |
| 0.250000 | 0.000000 | 0.409091 |
| 0.253501 | 0.991639 | 0.318124 |
| 0.250000 | 0.500000 | 0.409091 |
| 0.253230 | 0.492158 | 0.318267 |
| 0.750000 | 0.750000 | 0.454545 |
| 0.750616 | 0.748715 | 0.363759 |
| 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 $\Theta=0.50$ 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  | 0.250000 | 0.750000 | 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  | 0.729111 | 0.731377 | 0.772453 |
| Ti  | 0.269720 | 0.231142 | 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 0.252955 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 $\Theta=0.00$ 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 (x, y, z) | O (x, y, z) |
|------------|------------|
| 0.750000 0.250000 0.590909 | 0.250000 0.000000 0.500000 |
| 0.749359 0.250281 0.681444 | 0.250000 0.000000 0.500000 |
| 0.748946 0.250408 0.770417 | 0.250000 0.000308 0.681701 |
| 0.750000 0.750000 0.500000 | 0.249391 0.000446 0.771309 |
| 0.750000 0.750000 0.590909 | 0.750000 0.000000 0.500000 |
| 0.749344 0.750298 0.681445 | 0.750000 0.000000 0.500000 |
| 0.748918 0.750408 0.770423 | 0.750000 0.000000 0.500000 |
| 0.250000 0.250000 0.500000 | 0.249353 0.750319 0.318555 |
| 0.249388 0.750409 0.229576 | 0.249679 0.250093 0.636497 |
| 0.750000 0.250000 0.500000 | 0.249159 0.250432 0.727639 |
| 0.748938 0.750409 0.229576 | 0.249131 0.750345 0.727644 |
| 0.750000 0.750000 0.500000 | 0.249576 0.250233 0.636497 |
| 0.749344 0.750298 0.318555 | 0.249079 0.250339 0.727638 |
| 0.748918 0.750408 0.229576 | 0.750000 0.750000 0.545455 |
| 0.749353 0.750319 0.318555 | 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
0.998914 0.750939 0.228640
0.500000 0.250000 0.409091
0.499337 0.246261 0.318299
0.498940 0.250943 0.228641
0.500000 0.750000 0.409091
0.499320 0.754376 0.318310
0.498913 0.749954 0.228626
Structure 32. ZrO$_2$-terminated BaZrO$_3$ slab at $\Theta$=0.25 CO$_2$ coverage

```plaintext
_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
| X  | Y  | Z   |
|----|----|-----|
| 0  | 0.749169 | 0.250122 | 0.363659 |
| 0  | 0.750000 | 0.000000 | 0.409091 |
| 0  | 0.750000 | 0.500000 | 0.409091 |
| 0  | 0.000000 | 0.250000 | 0.409091 |
| 0  | 0.000000 | 0.750000 | 0.409091 |
| 0  | 0.500000 | 0.250000 | 0.409091 |
| 0  | 0.500000 | 0.750000 | 0.409091 |
| 0  | 0.250000 | 0.250000 | 0.454545 |
| 0  | 0.750000 | 0.250000 | 0.454545 |
| 0  | 0.750000 | 0.750000 | 0.454545 |
| 0  | 0.250000 | 0.000000 | 0.500000 |
| 0  | 0.250000 | 0.500000 | 0.500000 |
| 0  | 0.750000 | 0.000000 | 0.500000 |
| 0  | 0.000000 | 0.250000 | 0.500000 |
| 0  | 0.000000 | 0.750000 | 0.500000 |
| 0  | 0.500000 | 0.250000 | 0.500000 |
| 0  | 0.500000 | 0.750000 | 0.500000 |
| 0  | 0.250000 | 0.250000 | 0.545455 |
| 0  | 0.750000 | 0.250000 | 0.545455 |
| 0  | 0.750000 | 0.750000 | 0.545455 |
| 0  | 0.250000 | 0.000000 | 0.590909 |
| 0  | 0.250000 | 0.500000 | 0.590909 |
| 0  | 0.750000 | 0.000000 | 0.590909 |
| 0  | 0.750000 | 0.500000 | 0.590909 |
| 0  | 0.000000 | 0.250000 | 0.590909 |
| 0  | 0.000000 | 0.750000 | 0.590909 |
| 0  | 0.500000 | 0.250000 | 0.590909 |
| 0  | 0.500000 | 0.750000 | 0.590909 |
| 0  | 0.250571 | 0.250075 | 0.636341 |
| 0  | 0.749169 | 0.250122 | 0.636341 |
| 0  | 0.247114 | 0.750289 | 0.636595 |
| 0  | 0.752625 | 0.750246 | 0.636596 |
| 0  | 0.499752 | 0.754622 | 0.680812 |
| 0  | 0.253411 | 0.500268 | 0.681444 |
| 0  | 0.746042 | 0.500268 | 0.681457 |
| 0  | 0.754352 | 0.000517 | 0.681530 |
| 0  | 0.245097 | 0.000516 | 0.681543 |
| 0  | 0.999752 | 0.254467 | 0.681657 |
| 0  | 0.499751 | 0.246064 | 0.681954 |
| 0  | 0.999751 | 0.746362 | 0.683189 |
| 0  | 0.751564 | 0.251081 | 0.727052 |
Structure 33. ZrO$_2$-terminated BaZrO$_3$ slab at $\Theta=0.50$ 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 |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| 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   | 0.749456 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. HfO2-terminated BaHfO3 slab at Θ=0.00 CO2 coverage

_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  0.590909
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
| X | Y   | Z   |
|---|-----|-----|
| 0.751489 | 0.750958 | 0.727462 |
| 0.000000 | 0.250000 | 0.500000 |
| 0.001203 | 0.249739 | 0.681696 |
| 0.001869  | 0.251010 | 0.771583 |
| 0.000000 | 0.750000 | 0.500000 |
| 0.001211  | 0.751384 | 0.681714 |
| 0.001866  | 0.750774 | 0.771560 |
| 0.500000 | 0.250000 | 0.500000 |
| 0.500000 | 0.250000 | 0.500000 |
| 0.501208  | 0.251409 | 0.681706 |
| 0.501865  | 0.250785 | 0.771561 |
| 0.500000 | 0.750000 | 0.500000 |
| 0.500000 | 0.750000 | 0.500000 |
| 0.501214  | 0.749738 | 0.681693 |
| 0.501863  | 0.751007 | 0.771574 |
| 0.250000  | 0.000000 | 0.409091 |
| 0.252034  | 0.000568 | 0.318271 |
| 0.251754  | 0.000896 | 0.228465 |
| 0.250000  | 0.500000 | 0.409091 |
| 0.250369  | 0.500572 | 0.318324 |
| 0.251989  | 0.500893 | 0.228407 |
| 0.750000  | 0.000000 | 0.409091 |
| 0.750362  | 0.000583 | 0.318329 |
| 0.751974  | 0.000897 | 0.228390 |
| 0.750000  | 0.500000 | 0.409091 |
| 0.752014  | 0.500585 | 0.318262 |
| 0.751749  | 0.500893 | 0.228468 |
| 0.250000  | 0.250000 | 0.454545 |
| 0.250662  | 0.250217 | 0.363568 |
| 0.251476  | 0.250880 | 0.272540 |
| 0.250000  | 0.750000 | 0.454545 |
| 0.250643  | 0.750407 | 0.363567 |
| 0.251597  | 0.750564 | 0.272542 |
| 0.750000  | 0.250000 | 0.454545 |
| 0.750650  | 0.250431 | 0.363566 |
| 0.751593  | 0.250530 | 0.272537 |
| 0.750000  | 0.750000 | 0.454545 |
| 0.750682  | 0.750203 | 0.363565 |
| 0.751489  | 0.750958 | 0.272538 |
| 0.000000  | 0.250000 | 0.409091 |
| 0.001203  | 0.249739 | 0.318303 |
| 0.001869  | 0.251010 | 0.228417 |
| 0.000000  | 0.750000 | 0.409091 |
| 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 $\Theta$=0.25 CO$_2$ coverage

| parameter                      | value     |
|--------------------------------|-----------|
| 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 0.500890  0.500432  0.271100
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 0.500346  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  0.227849
Hf 0.767263  0.750869  0.227849
Hf 0.250438  0.250834  0.230531
Hf 0.751388  0.250836  0.230324
Hf 0.250135  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
C  0.501097  0.752135  0.197667
C  0.501097  0.752135  0.802333
O  0.364241  0.752448  0.186034
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
O  0.249569  0.501335  0.230048
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
O  0.000611  0.750705  0.317465
O  0.500585  0.250704  0.318201
O  0.000588  0.250301  0.318313
O  0.500605  0.750287  0.318405
O  0.250686  0.000640  0.318429
O  0.750478  0.000643  0.318435
O  0.750901  0.500411  0.318435
O  0.250260  0.500411  0.318462
O  0.249433  0.750317  0.363440
O  0.751205  0.750309  0.363442
O  0.250564  0.250237  0.363700
| O     | 0.250229 | 0.250947 | 0.726918 |
|-------|----------|----------|----------|
| O     | 0.745230 | 0.750612 | 0.728002 |
| O     | 0.256487 | 0.750573 | 0.728009 |
| O     | 0.752706 | 0.000548 | 0.769831 |
| O     | 0.249227 | 0.000528 | 0.769838 |
| O     | 0.752355 | 0.501349 | 0.769935 |
| 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 $\Theta=0.50$ CO$_2$ coverage

```plaintext
_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  0.000930  0.003889  0.272503  
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  0.000000  0.500000  0.636454  
Ba  0.500000  0.500000  0.636454  
Ba  0.000000  0.000000  0.636455  
Ba  0.000000  0.500000  0.636455  
Ba  0.500000  0.000000  0.636455  
Ba  0.500000  0.500000  0.636455  
Ba  0.250000  0.250000  0.409091  
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
```
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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   | 0.500000   | 0.409091   |
| Hf      | 0.750000   | 0.500000   | 0.409091   |
| Hf      | 0.250000   | 0.500000   | 0.500000   |
| Hf      | 0.750000   | 0.500000   | 0.500000   |
| C       | 0.000980   | 0.250947   | 0.198425   |
| C       | 0.500977   | 0.750938   | 0.198426   |
| C       | 0.500977   | 0.750938   | 0.801574   |
| C       | 0.000980   | 0.250947   | 0.801575   |
| O       | 0.864091   | 0.251008   | 0.186909   |
| O       | 0.364080   | 0.750996   | 0.186910   |
| O       | 0.637895   | 0.750968   | 0.186914   |
| O       | 0.137906   | 0.250981   | 0.186914   |
| O       | 0.000955   | 0.250773   | 0.228225   |
| O       | 0.500951   | 0.750772   | 0.228226   |
| O       | 0.000942   | 0.750387   | 0.228592   |
| O       | 0.500944   | 0.250389   | 0.228593   |
| O       | 0.751060   | 0.000617   | 0.231311   |
| O       | 0.251061   | 0.500618   | 0.231315   |
| O       | 0.250730   | 0.000616   | 0.231325   |
| O       | 0.750730   | 0.500616   | 0.231326   |
| O       | 0.757727   | 0.250486   | 0.272601   |
| O       | 0.257713   | 0.750502   | 0.272602   |
| O       | 0.244099   | 0.250573   | 0.272604   |
| O       | 0.744108   | 0.750587   | 0.272604   |
| O       | 0.500790   | 0.251213   | 0.317439   |
| O       | 0.000789   | 0.751215   | 0.317443   |
| O       | 0.500786   | 0.749729   | 0.318560   |
| O       | 0.000786   | 0.249727   | 0.318561   |
| O       | 0.751593   | 0.500449   | 0.318566   |
| O       | 0.251592   | 0.000450   | 0.318570   |
| O       | 0.250993   | 0.500450   | 0.318585   |
| X   | Y   | Z   |
|-----|-----|-----|
| 0.750094 | 0.000450 | 0.318587 |
| 0.749328 | 0.250286 | 0.363594 |
| 0.249337 | 0.750276 | 0.363595 |
| 0.251481 | 0.250208 | 0.363596 |
| 0.751470 | 0.750194 | 0.363596 |
| 0.250000 | 0.500000 | 0.409091 |
| 0.750000 | 0.000000 | 0.409091 |
| 0.250000 | 0.000000 | 0.409091 |
| 0.750000 | 0.500000 | 0.409091 |
| 0.000000 | 0.250000 | 0.409091 |
| 0.000000 | 0.750000 | 0.409091 |
| 0.500000 | 0.750000 | 0.409091 |
| 0.500000 | 0.250000 | 0.409091 |
| 0.750000 | 0.250000 | 0.454545 |
| 0.750000 | 0.750000 | 0.454545 |
| 0.250000 | 0.750000 | 0.454545 |
| 0.250000 | 0.250000 | 0.454545 |
| 0.250000 | 0.000000 | 0.500000 |
| 0.250000 | 0.500000 | 0.500000 |
| 0.750000 | 0.000000 | 0.500000 |
| 0.750000 | 0.500000 | 0.500000 |
| 0.000000 | 0.250000 | 0.500000 |
| 0.000000 | 0.750000 | 0.500000 |
| 0.500000 | 0.250000 | 0.500000 |
| 0.500000 | 0.750000 | 0.500000 |
| 0.250000 | 0.250000 | 0.545455 |
| 0.250000 | 0.750000 | 0.545455 |
| 0.750000 | 0.250000 | 0.545455 |
| 0.750000 | 0.750000 | 0.545455 |
| 0.250000 | 0.000000 | 0.590909 |
| 0.250000 | 0.500000 | 0.590909 |
| 0.750000 | 0.000000 | 0.590909 |
| 0.750000 | 0.500000 | 0.590909 |
| 0.000000 | 0.250000 | 0.590909 |
| 0.000000 | 0.750000 | 0.590909 |
| 0.500000 | 0.250000 | 0.590909 |
| 0.500000 | 0.750000 | 0.590909 |
| 0.251481 | 0.250208 | 0.636404 |
| 0.751470 | 0.750194 | 0.636404 |
| 0.249337 | 0.750276 | 0.636405 |
| 0.749328 | 0.250286 | 0.636406 |
| 0.750094 | 0.000450 | 0.681413 |
| 0.250093 | 0.500450 | 0.681415 |
| 0.251592 | 0.000450 | 0.681430 |
| 0.751593 | 0.500449 | 0.681434 |
| 0.000786 | 0.249727 | 0.681439 |
|   |   |   |   |
|---|---|---|---|
| O 0.500786 0.749729 0.681440 |
| O 0.000789 0.751215 0.682557 |
| O 0.500790 0.251213 0.682561 |
| O 0.244099 0.250573 0.727396 |
| O 0.744108 0.750587 0.727396 |
| O 0.257713 0.750502 0.727398 |
| O 0.757727 0.250486 0.727399 |
| O 0.750730 0.500616 0.768674 |
| O 0.250730 0.000616 0.768675 |
| O 0.251061 0.500618 0.768685 |
| O 0.751060 0.000617 0.768689 |
| O 0.500944 0.250389 0.771407 |
| O 0.000942 0.750387 0.771408 |
| O 0.500951 0.750772 0.771774 |
| O 0.000955 0.250773 0.771775 |
| O 0.637895 0.750968 0.813086 |
| O 0.137906 0.250981 0.813086 |
| O 0.364080 0.750996 0.813090 |
| O 0.864091 0.251008 0.813091 |