Electronic Supplementary Information

First Principles Studies of CO_2 and O_2 Chemisorption on La_2O_3 Surfaces

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This supplementary information is divided into two sections, briefly summarized below.

Section 1: Additional figures:

Figure S1. An Additional CO_2 Chemisorption Structure and Energy for the $La_2O_3(011)$ Surface Closely Related to the (011)-**II** Structure in Figure 3.

Figure S2. CO_2 Chemisorption Structures and Energies for the p(2×2) Supercells of the $La_2O_3(011)$, (100), (110), (101), and (111) Surfaces.

Figure S3. Phase Diagrams (T/K vs. p_{CO2}/bar) for the $La_2O_3(011)$, (100), (110), (101), and (111) Surfaces.

Figure S4. Additional O_2 Chemisorption Structures and Energies for the La_2O_3 Surfaces Related to Those in Figure 6.

Figure S5. O_2 Chemisorption Structures and Energies for the p(2×2) Supercells of the La_2O_3(011), (100), (110), (101), and (111) Surfaces.

Figure S6. Additional O_2 Chemisorption Structures and Energies for the p(2×2) Supercells of the La_2O_3(011), (100), (110), (101), and (111) Surfaces.

Figure S7. Calculated Band Structures for Bulk La_2O_3 and Its (001), (011), (100), (110), (101), and (111) Surfaces.

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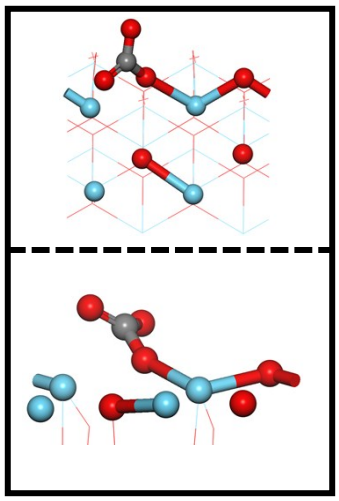
Figure S1. An Additional CO_2 Chemisorption Structure and Energy (eV) for the $La_2O_3(011)$ Surface Calculated at the PBE Level, Which Is Closely Related to the (011)-**II** Structure in Figure 3.



(011)-**III**: −1.02

Figure S2. CO_2 Chemisorption Structures and Energies (eV) for the p(2×2) Supercells of the La_2O_3(011), (100), (110), (101), and (111) Surfaces Calculated at the PBE Level. The Labels of These Structures Correspond to Those in Figures 3 and S1, with Additional Structures Labeled with Higher Numbers.

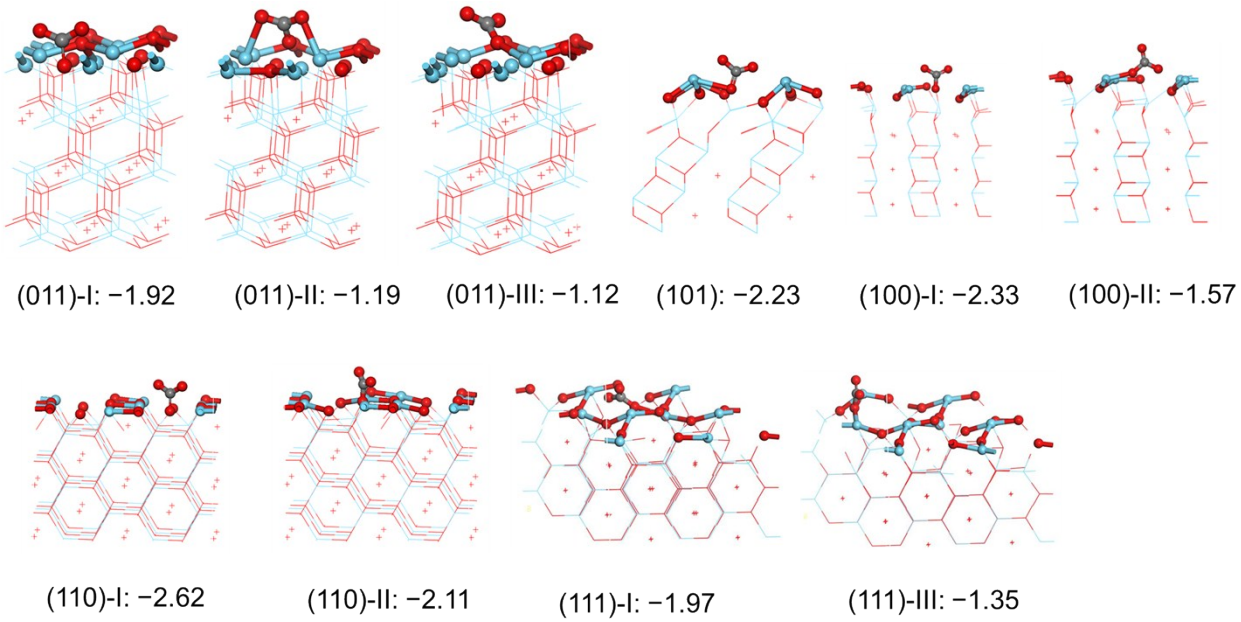


Figure S3. Phase diagrams (T/K vs. p_{CO2}/bar) for the La_2O_3(011), (100), (110), (101), and (111) surfaces (Figure 1, blue) in equilibrium with the carbonate-covered (011)-**I**, (100), (110)-**I**, and (101)-**I** surfaces (0.5−1 ML, Figure 3, red; 0.25 ML, Figure S2, green) under the CO_2 environment.

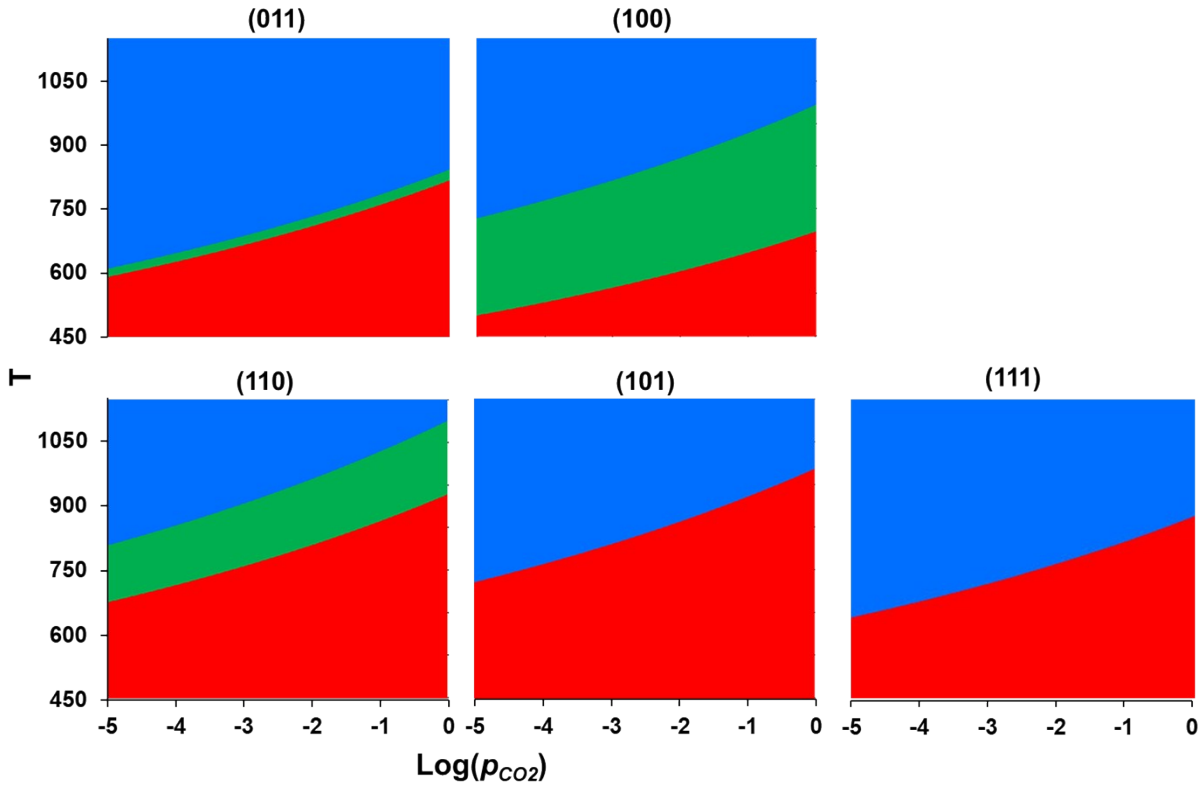


Figure S4. Additional O_2 Chemisorption Structures and Energies (eV) for the La_2O_3 Surfaces Calculated at the PBE Level, Which Are Related to Those in Figure 6. The (011)-**III** Structure, Which Is Closely Related to (011)-**I** Structure, Was Predicted to Be Lower in Energy than the (011)-**II** Structure in Figure 6.

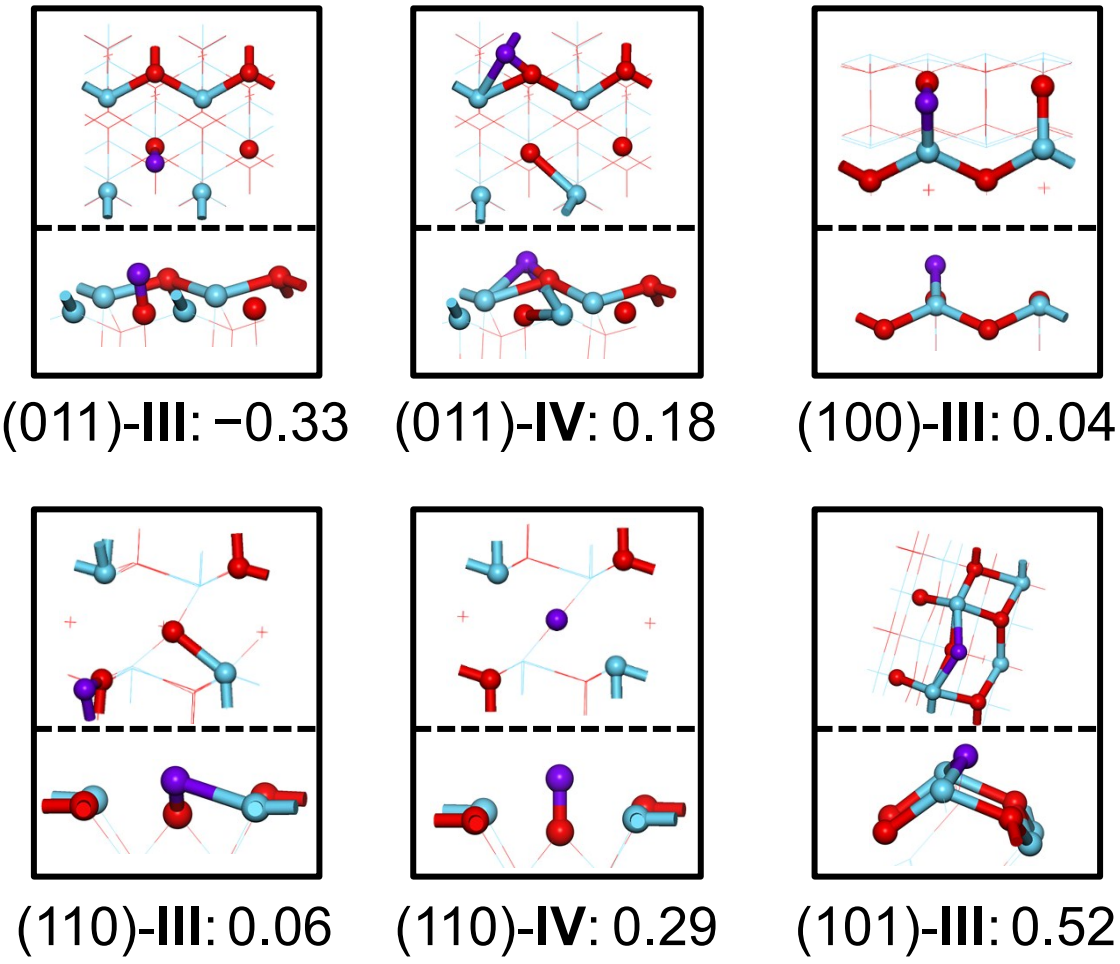


Figure S5. O_2 Chemisorption Structures and Energies (eV) for the p(2×2) Supercells of the La_2O_3(011), (100), (110), (101), and (111) Surfaces Calculated at the PBE Level. The Labels of These Structures Correspond to Those in Figures 6.

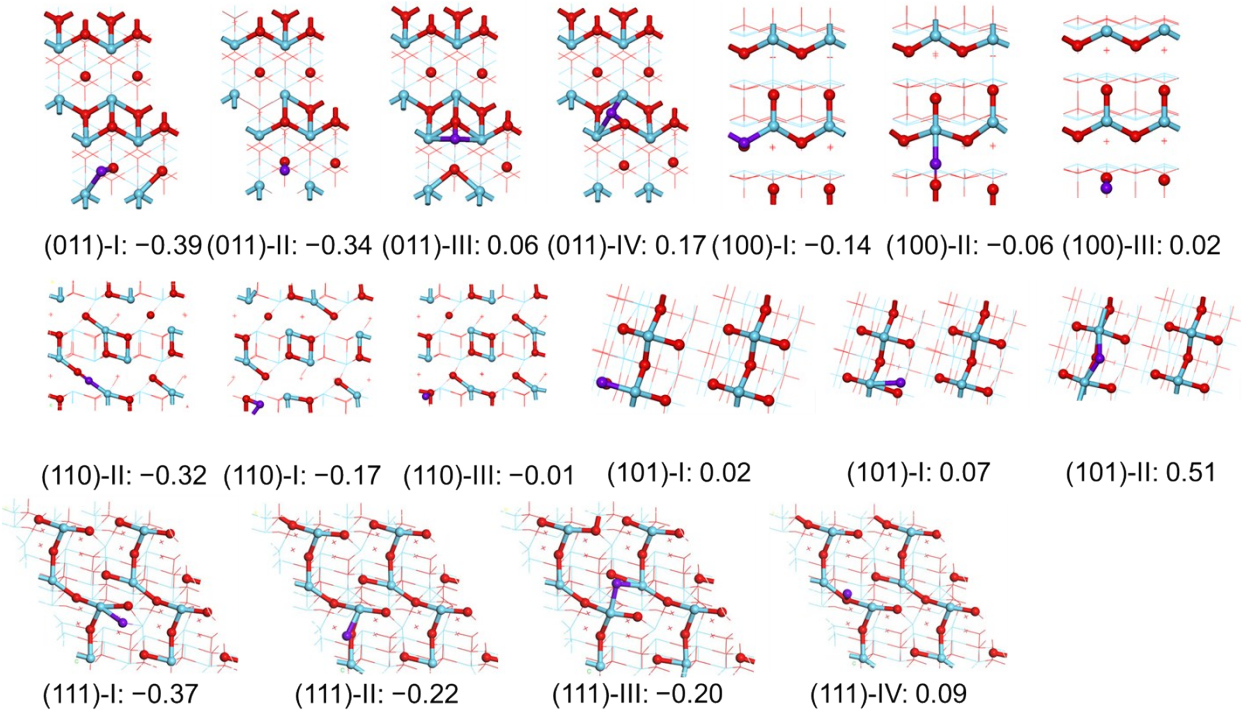
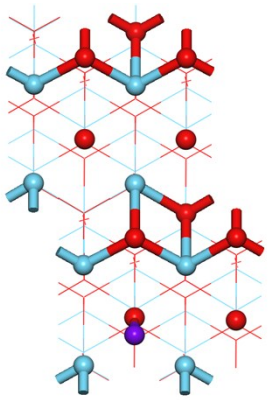
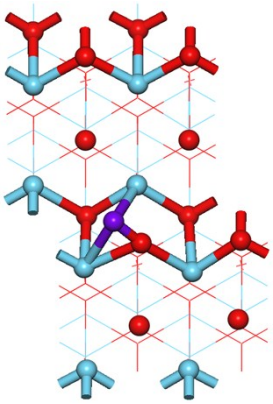


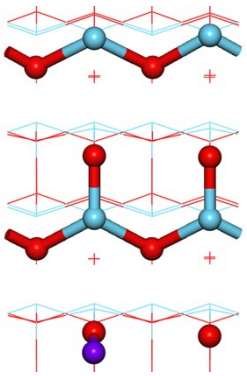
Figure S6. Additional O_2 Chemisorption Structures and Energies (eV) for the p(2×2) Supercells of the La_2O_3(011), (100), (110), and (101) Surfaces Calculated at the PBE Level. The Labels of These Structures Correspond to Those in Figures S4, with Additional Structures Labeled with Higher Numbers.



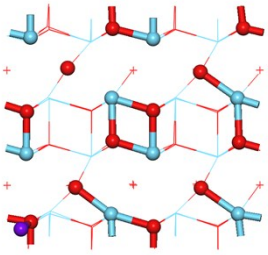
(011)-**III**: -0.34



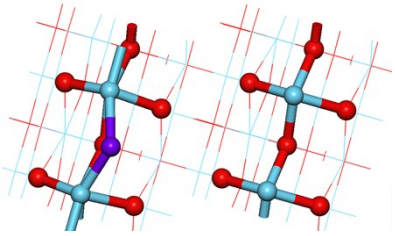
(011)-**IV**: 0.17



(100)-**III**: 0.02

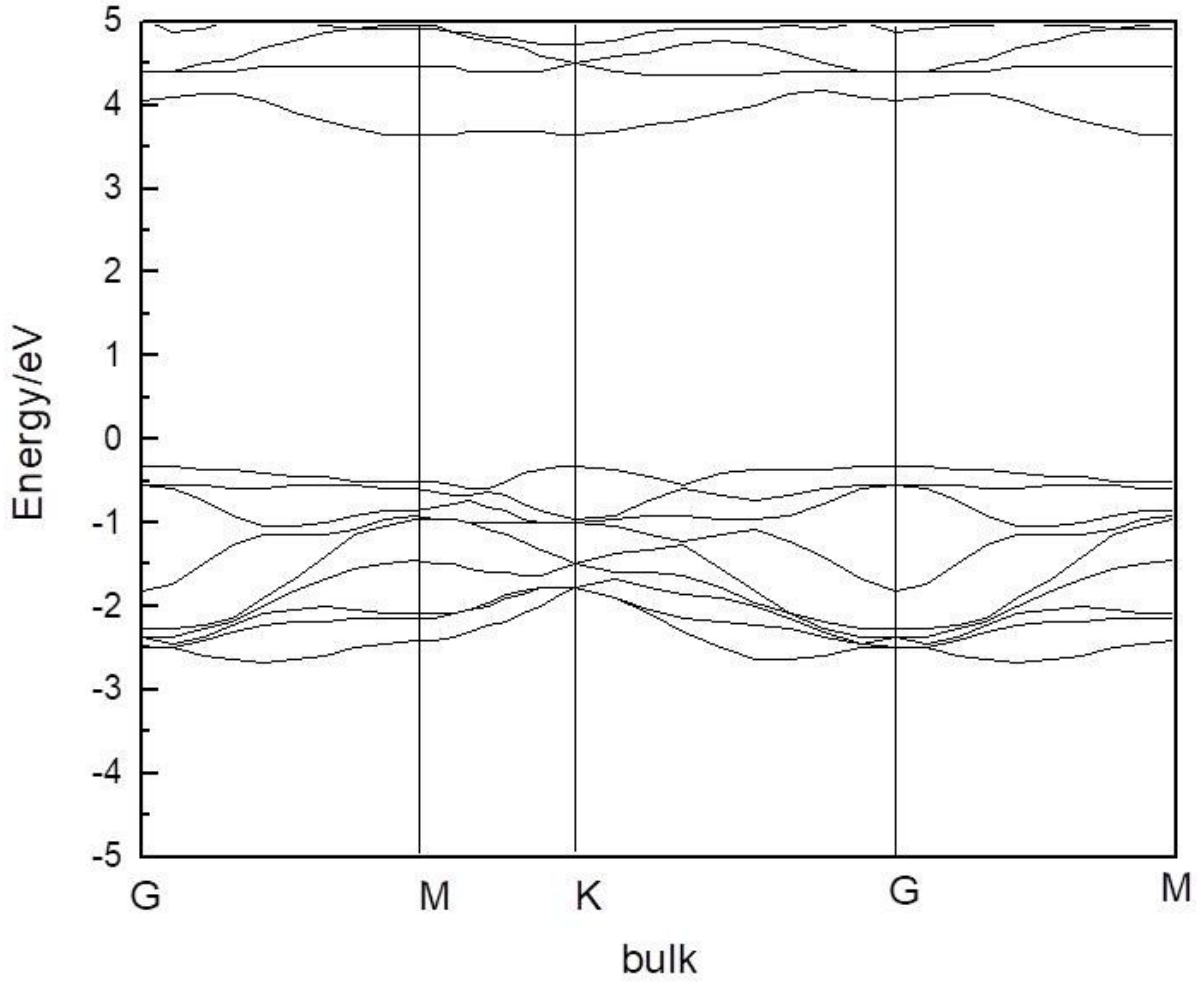


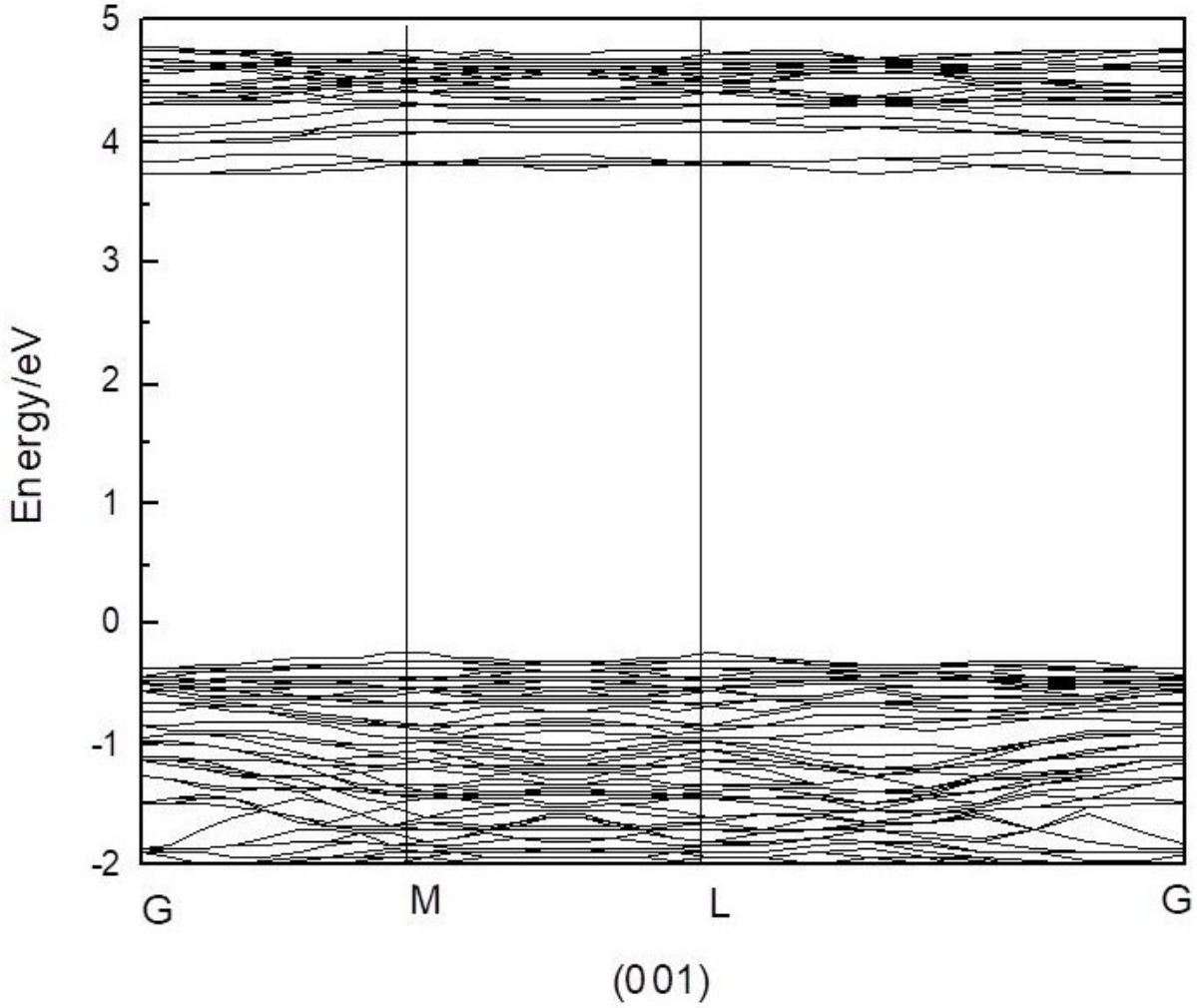
(110)-**III**: -0.01

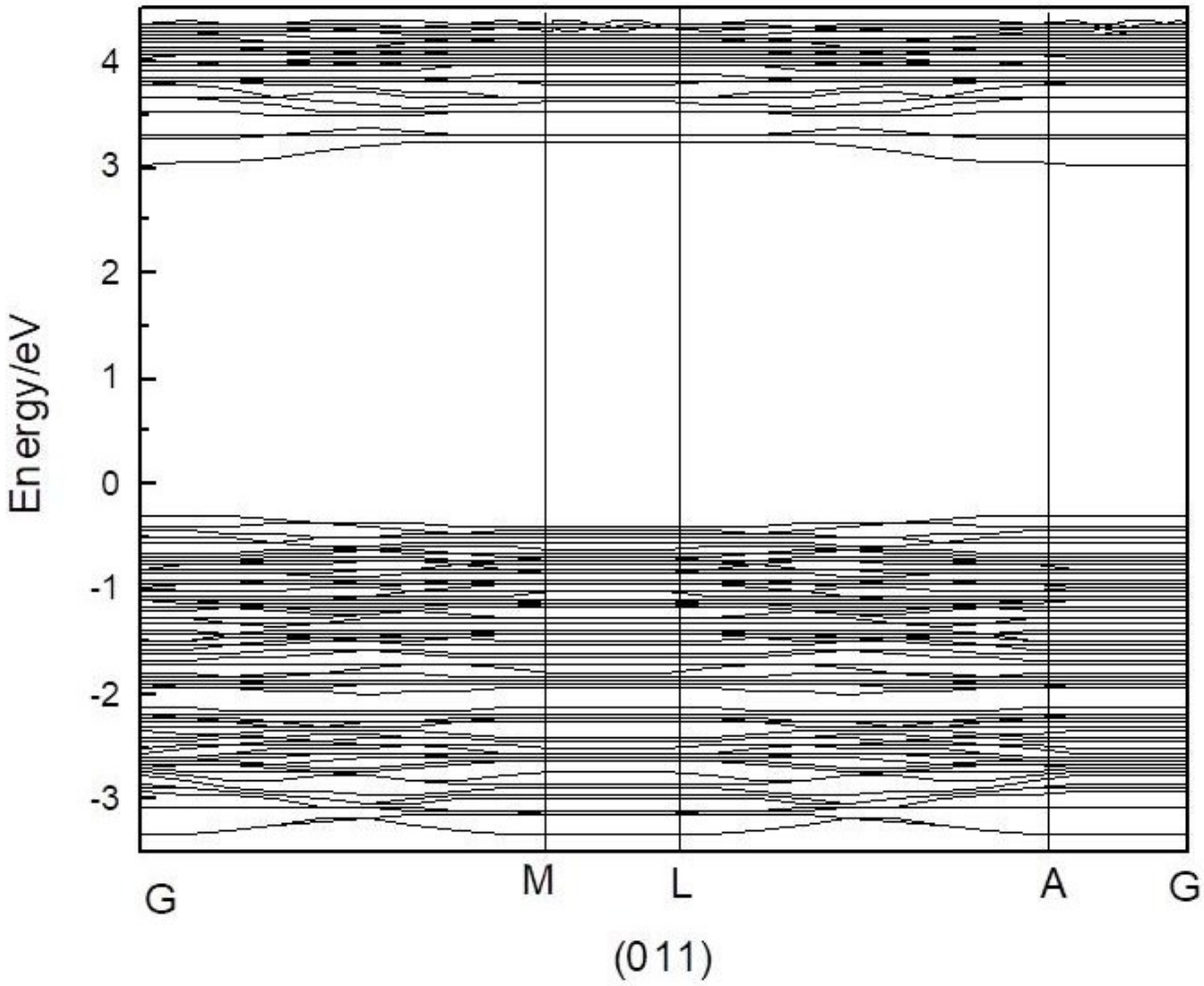


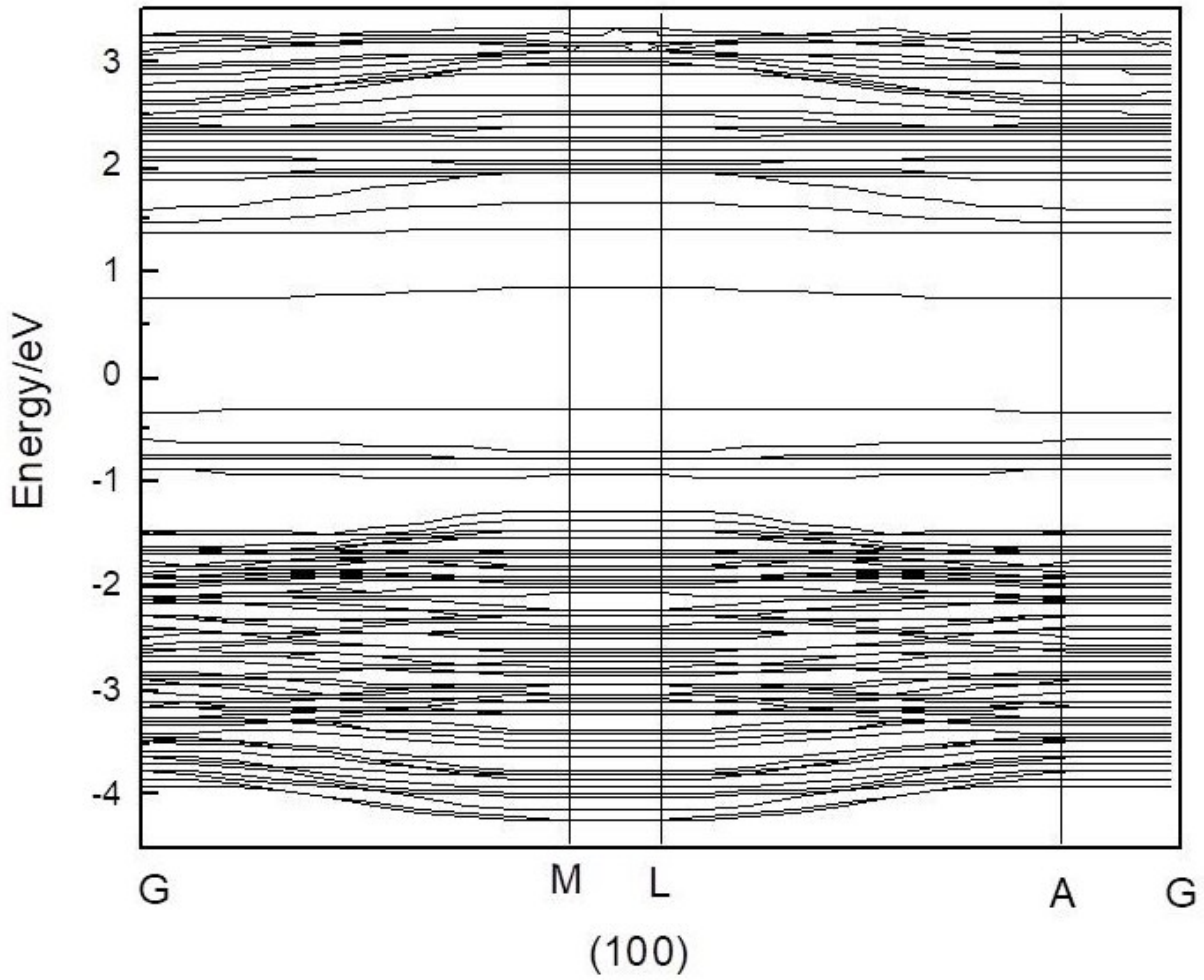
(101)-**III**: 0.51

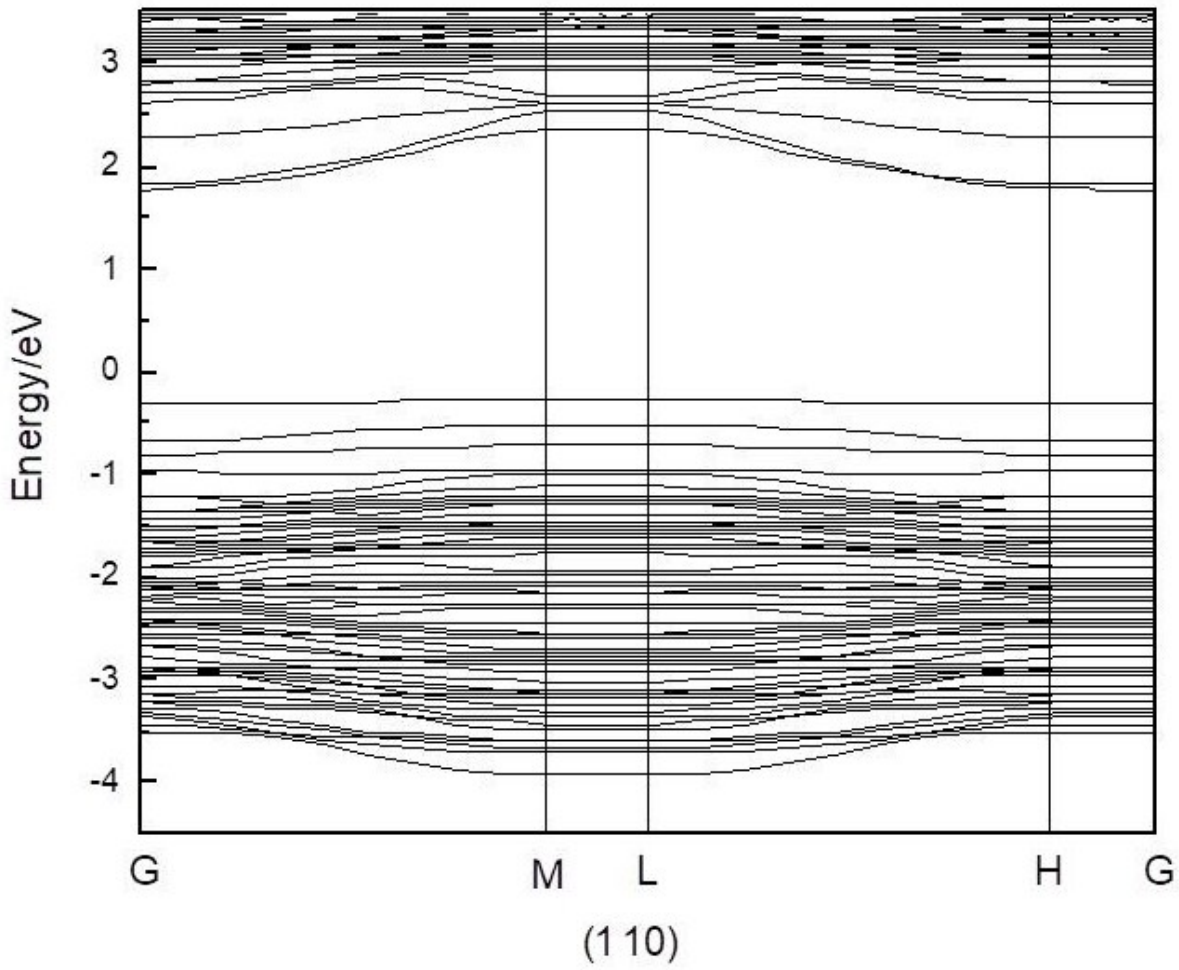
Figure S7. Calculated Band Structures for Bulk La_2O_3 and Its (001), (011), (100), (110), (101), and (111) Surfaces.

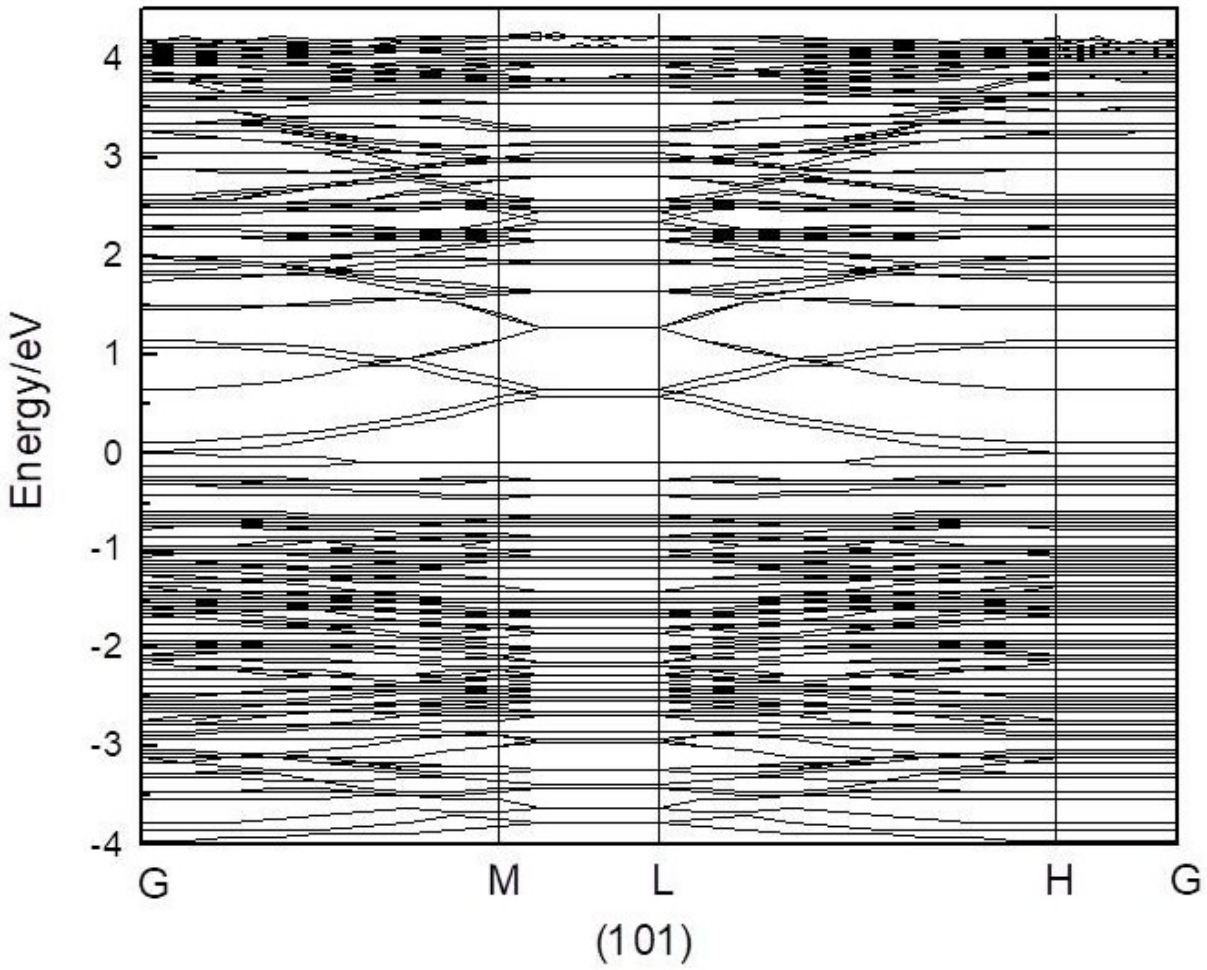


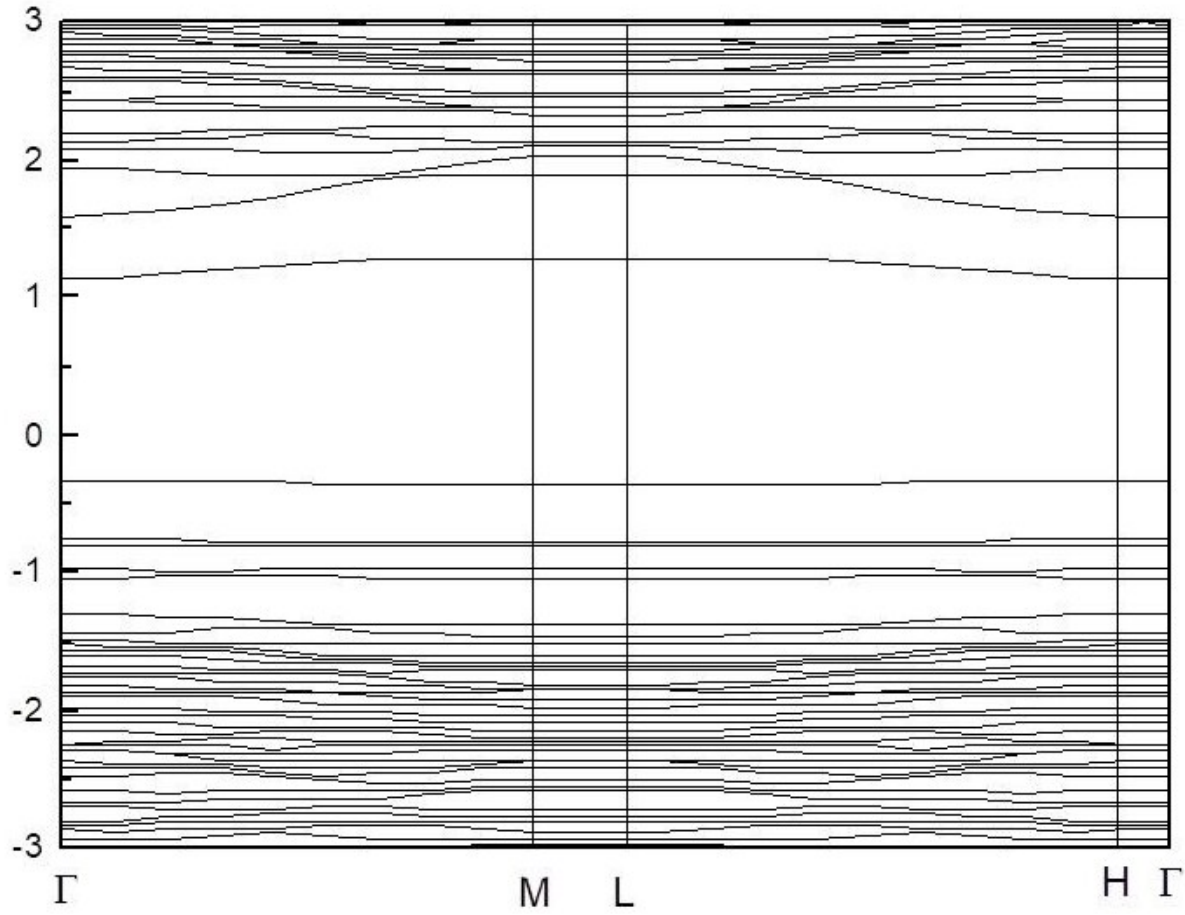

5
4
3
2
1
0
-1
-2
Energy/eV
G
M
L
G
(001)


Energy/eV
4
3
2
1
0
-1
-2
-3
G
M
L
A
G
(011)


Energy/eV
3
2
1
0
-1
-2
-3
-4
G
M
L
A
G
(100)


Energy/eV
3
2
1
0
-1
-2
-3
-4
G
M
L
H
G
(1 10)


Energy/eV
4
3
2
1
0
-1
-2
-3
-4
G
M
L
H
G
(101)



(111)

Table S1. Optimization of the Number of Repeating Units Based on the Calculated O_2 Dissociation Energies with the p(1×1) Unit Cell.

Number of Repeating Units	Structure 1	Structure 2	Structure 3	Structure 4
(001)				
2	0.265			
4	0.266			
6	0.266			
(011)				
2	−0.267	−0.182	0.105	0.327
4	−0.368	−0.318	0.136	0.320
6	−0.361	−0.312	0.136	0.321
(100)				
2	−0.132	−0.079	0.111	
4	−0.104	−0.067	0.168	
6	−0.107	−0.067	0.171	
(110)				
2	0.474	0.468	0.757	
4	0.007	0.094	0.294	
6	−0.014	0.057	0.292	
8	−0.015	0.059	0.297	
(101)				
2	0.148	0.205	0.859	
4	0.165	0.285	0.626	
6	0.159	0.282	0.618	
(111)				
4	−0.364	−0.172	−0.091	0.189
6	−0.363	−0.206	−0.126	0.139
8	−0.356	−0.245	−0.134	0.141

Table S2. Optimized Fractional Coordinates of Bulk La_2O_3 and Its Surfaces Shown in Figure 1.

La_2O_3 Bulk

```
La  O
   1.00000000000000
     3.4116974049199555   -1.9697444151240839   -0.0000000000000000
     0.0000000000000000    3.9394888302481679    0.0000000000000000
    -0.0000000000000000    0.0000000000000000    6.1838024734529302
   La   O
     2     3
Direct
  0.3333333333333357  0.6666666666666643  0.2473852580061383
  0.6666666666666643  0.3333333333333357  0.7526147419938617
  0.0000000000000000 -0.0000000000000000  0.0000000000000000
  0.3333333333333357  0.6666666666666643  0.6454421768759356
  0.6666666666666643  0.3333333333333357  0.3545578231240644
```

Figure 1(a): La_2O_3(001), p(2×2)

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    24    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.0000000000000000  0.0000000000000000  0.6206837706312953   T   T   T
  0.1666666666666714  0.3333333333333286  0.5352302760047607   T   T   T
  0.3333333333333286  0.1666666666666714  0.7050789635715589   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.0000000000000000  0.5000000000000000  0.6206837706312953   T   T   T
  0.1666666666666714  0.8333333333333357  0.5352302760047607   T   T   T
  0.3333333333333357  0.6666666666666714  0.7050789635715589   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.5000000000000000  0.0000000000000000  0.6206837706312953   T   T   T
  0.6666666666666714  0.3333333333333286  0.5352302760047607   T   T   T
  0.8333333333333286  0.1666666666666714  0.7050789635715589   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.5000000000000000  0.5000000000000000  0.6206837706312953   T   T   T
  0.6666666666666714  0.8333333333333357  0.5352302760047607   T   T   T
  0.8333333333333286  0.6666666666666714  0.7050789635715589   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
```

```
  0.1666666666666714  0.3333333333333286  0.6810249590977548   T   T   T
  0.3333333333333286  0.1666666666666714  0.5612805770190477   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1666666666666714  0.8333333333333357  0.6810249590977548   T   T   T
  0.3333333333333357  0.6666666666666714  0.5612805770190477   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6666666666666714  0.3333333333333286  0.6810249590977548   T   T   T
  0.8333333333333286  0.1666666666666714  0.5612805770190477   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6666666666666714  0.8333333333333357  0.6810249590977548   T   T   T
  0.8333333333333286  0.6666666666666714  0.5612805770190477   T   T   T
```

Figure 1(b): La_2O_3(011), p(2×1)

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    24    16
Selective dynamics
Direct
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0209463572325674  0.0837854289302697  0.5627620831423386   T   T   T
  0.1299444777812155  0.5197779111248479  0.5947003353976115   T   T   T
  0.4152800144615441  0.6611200578461620  0.5213594595512276   T   T   T
  0.3238122028332384  0.2952488113329466  0.6655198830799591   T   T   T
  0.4378515926514197  0.7514063706056575  0.7065011146738698   T   T   T
  0.2217328727110655  0.8869314908442618  0.6365382435538365   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5209463572325674  0.0837854289302697  0.5627620831423386   T   T   T
  0.6299444777812155  0.5197779111248479  0.5947003353976115   T   T   T
  0.9152800144615441  0.6611200578461620  0.5213594595512276   T   T   T
  0.8238122028332384  0.2952488113329466  0.6655198830799591   T   T   T
  0.9378515926514197  0.7514063706056575  0.7065011146738698   T   T   T
  0.7217328727110655  0.8869314908442618  0.6365382435538365   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2045332244869513  0.8181328979478124  0.5478162324360270   T   T   T
  0.3388184684896132  0.3552738739584527  0.5697677224578115   T   T   T
  0.0122838765151556  0.0491355060606082  0.6612419757357912   T   T   T
```

```
  0.1494675664277452  0.5978702657109949  0.6830634168174470   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7045332244869513  0.8181328979478124  0.5478162324360270   T   T   T
  0.8388184684896132  0.3552738739584527  0.5697677224578115   T   T   T
  0.5122838765151556  0.0491355060606082  0.6612419757357912   T   T   T
  0.6494675664277452  0.5978702657109949  0.6830634168174470   T   T   T
```

Figure 1(c): La_2O_3(100), p(2×1)

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.5095608658341177
   O    La
    24    16
Selective dynamics
Direct
  0.3750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.1250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.1250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.1250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.3750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.3750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.3750000000000000  0.5101956642992533  0.5576528012902244   T   T   T
  0.1250000000000000  0.1535363141919177  0.6078795815743092   T   T   T
  0.1250000000000000  0.8622295020693755  0.5209432937096565   T   T   T
  0.1250000000000000  0.5577280848488684  0.6883056474959304   T   T   T
  0.3750000000000000  0.0685890119316568  0.7269487361905504   T   T   T
  0.3750000000000000  0.8400826252327320  0.6411935283526233   T   T   T
  0.8750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.6250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.6250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.6250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.8750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.8750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.8750000000000000  0.5101956642992533  0.5576528012902244   T   T   T
  0.6250000000000000  0.1535363141919177  0.6078795815743092   T   T   T
  0.6250000000000000  0.8622295020693755  0.5209432937096565   T   T   T
  0.6250000000000000  0.5577280848488684  0.6883056474959304   T   T   T
  0.8750000000000000  0.0685890119316568  0.7269487361905504   T   T   T
  0.8750000000000000  0.8400826252327320  0.6411935283526233   T   T   T
  0.1250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.1250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.3750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.3750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.1250000000000000  0.7332447342073536  0.6004183617653354   T   T   T
  0.1250000000000000  0.2515567820036182  0.5213274067156419   T   T   T
  0.3750000000000000  0.7257421713467167  0.7195314323197195   T   T   T
  0.3750000000000000  0.2215794469269170  0.6528683418881656   T   T   T
  0.6250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.6250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.8750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.8750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
```

```
  0.6250000000000000  0.7332447342073536  0.6004183617653354   T   T   T
  0.6250000000000000  0.2515567820036182  0.5213274067156419   T   T   T
  0.8750000000000000  0.7257421713467167  0.7195314323197195   T   T   T
  0.8750000000000000  0.2215794469269170  0.6528683418881656   T   T   T
```

Figure 1(d): La_2O_3(110), p(1×1)

```
O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   O    La
    18    12
Selective dynamics
Direct
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.5000000000000000  0.5000000000000000  0.5371347587154673   T   T   T
  0.8367698155022723  0.8498590053713997  0.5389868928471344   T   T   T
  0.1632301844977277  0.1501409946286003  0.5389868928471344   T   T   T
  0.0000000000000000  0.5000000000000000  0.6287446622640616   T   T   T
  0.3244361859531466  0.8613473411541506  0.6190640561905880   T   T   T
  0.6755638140468534  0.1386526588458494  0.6190640561905880   T   T   T
  0.5000000000000000  0.5000000000000000  0.6801360352225529   T   T   T
  0.8415679729295107  0.8645680076307656  0.7000063927747959   T   T   T
  0.1584320270704893  0.1354319923692344  0.7000063927747959   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8313274659844865  0.2483512966935280  0.5379894754827177   T   T   T
  0.1686725340155135  0.7516487033064720  0.5379894754827177   T   T   T
  0.3324153020609231  0.2594651218275956  0.6225903589867627   T   T   T
  0.6675846979390769  0.7405348781724044  0.6225903589867627   T   T   T
  0.8329891729758074  0.2377469817433351  0.6939405913343819   T   T   T
  0.1670108270241926  0.7622530182566649  0.6939405913343819   T   T   T
```

Figure 1(e): La_2O_3(101), p(1×2)

```
O  La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   O    La
    24    16
Selective dynamics
Direct
```

```
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.0945824452507011  0.4763683352071668  0.5597763478321337   T   T   T
  0.4414902833905449  0.1396626976348886  0.5492664809194773   T   T   T
  0.7447098985454413  0.3138468152925813  0.5626242243004430   T   T   T
  0.3315138107972794  0.1671807031764188  0.6565948306992762   T   T   T
  0.6314513150237464  0.3422031763014593  0.6706271311533920   T   T   T
  0.9013447646556004  0.0247339892838942  0.6772399671884796   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.0945824452507011  0.9763683352071669  0.5597763478321337   T   T   T
  0.4414902833905449  0.6396626976348885  0.5492664809194773   T   T   T
  0.7447098985454413  0.8138468152925816  0.5626242243004430   T   T   T
  0.3315138107972794  0.6671807031764191  0.6565948306992762   T   T   T
  0.6314513150237464  0.8422031763014596  0.6706271311533920   T   T   T
  0.9013447646556004  0.5247339892838940  0.6772399671884796   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7415372075469049  0.0646294654155790  0.5101202495644676   T   T   T
  0.4121628623943770  0.3969930862490161  0.5988508970346734   T   T   T
  0.9632966302007805  0.2592491854333706  0.6308231755242097   T   T   T
  0.5944235915244526  0.1014645383520807  0.7059680284256874   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7415372075469049  0.5646294654155790  0.5101202495644676   T   T   T
  0.4121628623943770  0.8969930862490161  0.5988508970346734   T   T   T
  0.9632966302007805  0.7592491854333704  0.6308231755242097   T   T   T
  0.5944235915244526  0.6014645383520805  0.7059680284256874   T   T   T
```

Figure 1(f): $La_2O_3(111)$, p(1×1)

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O
    12    18
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5495114567158340  0.5272806903374965  0.2654242942143138   T   T   T
  0.0667706451959089  0.5613761907268492  0.3561788390254257   T   T   T
```

0.6547722425131486	0.7868463960819829	0.3987796245260316	T	T	T
0.4800332923790691	0.7044706516406336	0.0078164495430713	F	F	F
0.0260606697731873	0.7966127010022035	0.0808088664203765	F	F	F
0.5721759798694777	0.8887547503637734	0.1538012832976889	F	F	F
0.1081579732430205	0.9742499266649941	0.2236875193714255	T	T	T
0.6513882635254015	0.0669398218433470	0.2942684292915018	T	T	T
0.2021933237959167	0.1080713403334657	0.3707919674826757	T	T	T
0.7009704423389636	0.4798166249363334	0.0258603927668659	F	F	F
0.2469978197330818	0.5719586742979033	0.0988528096441783	F	F	F
0.7931131298293721	0.6641007236594731	0.1718452265214836	F	F	F
0.3715498932347884	0.7586456595586883	0.2385464034598553	T	T	T
0.8198093670207072	0.8350917199858329	0.3122942078433298	T	T	T
0.3946593862267554	0.8891549129236551	0.3663754356333918	T	T	T
0.1953125813377383	0.8018515466180745	0.0000000000000000	F	F	F
0.7413508490531768	0.8938395122850622	0.0729924168773124	F	F	F
0.2873782264472950	0.9859815616466321	0.1459848337546177	F	F	F
0.8421611165800051	0.0899619994067352	0.2156312136915643	T	T	T
0.3569149194094840	0.1660739910540391	0.2903499028048342	T	T	T
0.9046964424376301	0.1900639543542088	0.3746643002062875	T	T	T
0.2067639675224910	0.1579357869491815	0.0517596733424099	F	F	F
0.7527327231151588	0.2500778363107514	0.1247520902197152	F	F	F
0.2989066550128996	0.3422198856723213	0.1977445070970276	F	F	F
0.8543449252558765	0.4394500835916654	0.2771542189410545	T	T	T
0.3884604156902667	0.4841144985105553	0.3639997928622698	T	T	T
0.9629998411377750	0.7576101334463674	0.4121292247893837	T	T	T

Table S3. Optimized Fractional Coordinates for the Stationary States Shown in Figure 2.

Figure 2. CO_2 Physisorption

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.4183898508924397  0.6171047220299419  0.8060881038822226   T   T   T
  0.2692491624839419  0.4697126484326265  0.8114986064033306   T   T   T
  0.5709661589126072  0.7629879353044605  0.8032322712896367   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0012347386105390  0.0004290552847564  0.6207714485068391   T   T   T
  0.1663197292295357  0.3332646653495613  0.5349917275465933   T   T   T
  0.3336349898556858  0.1672878464747538  0.7047847595393232   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0012883599029697  0.5022262929962376  0.6196778708245896   T   T   T
  0.1666194913006173  0.8336135324936003  0.5349350351444783   T   T   T
  0.3329329487711525  0.6669369466047770  0.7045406064787604   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6666972770761177  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4982922299463516  0.0006762373176283  0.6202473434572346   T   T   T
  0.6670383212401380  0.3334712262920008  0.5349735097116001   T   T   T
  0.8333569205873805  0.1682527805458320  0.7033806835670561   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.4995515221975785  0.4983434936937939  0.6201925299762698   T   T   T
  0.6669392769634865  0.8338628441532246  0.5351945265370108   T   T   T
  0.8334872970696401  0.6668076581055311  0.7041321308216978   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1660773432425797  0.3324745156779603  0.6806832568883618   T   T   T
  0.3336082186032275  0.1671048223089586  0.5609212048262194   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1665103830134251  0.8347015853096769  0.6798516379189186   T   T   T
  0.3330605314905632  0.6666859861044132  0.5611427167878971   T   T   T
  0.6666972770761177  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6656986347238650  0.3340195351694003  0.6798832169241239   T   T   T
  0.8334797923869292  0.1670957474504814  0.5610539851239118   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6685895990804059  0.8355541316314693  0.6813137651190988   T   T   T
  0.8334292559111011  0.6667511136923816  0.5610141201958914   T   T   T
```

Figure 2. CO_2 Transitional State

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.4016404851692776  0.6131805696442343  0.7846950797307570   T   T   T
  0.2601137530623114  0.4588724673922685  0.7939029467202887   T   T   T
  0.5598124690683943  0.7543691811877214  0.7906072440637915   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790859498024091   F   F   F
  0.1666477117881300  0.3332954235762315  0.2933258797492897   F   F   F
  0.3333418362248537  0.1666477117881300  0.4648242920125725   F   F   F
  0.0009304364964970  1.0008424837598864  0.6208061842890715   T   T   T
  0.1657704691595555  0.3317328014076578  0.5347870821065253   T   T   T
  0.3346294900336286  0.1660947119744351  0.7033945394867066   T   T   T
  0.9999942969546183  0.5000245545708069  0.3790859498024091   F   F   F
  0.1666420087427483  0.8333199781470384  0.2933258797492897   F   F   F
  0.3333361331794720  0.6666722663589084  0.4648242920125725   F   F   F
  0.0092276343901553  0.5058530576155964  0.6201061900238724   T   T   T
  0.1658526644114965  0.8341624130939725  0.5349053820162033   T   T   T
  0.3329785519778669  0.6680310568403893  0.7075629272684540   T   T   T
  0.4999654495604560  0.0000000000000000  0.3790859498024091   F   F   F
  0.6666836724497003  0.3332954235762315  0.2933258797492897   F   F   F
  0.8333072857853026  0.1666477117881300  0.4648242920125725   F   F   F
  0.4943893597569460  0.9923510029039053  0.6204032946073692   T   T   T
  0.6670456416222815  0.3333961511797386  0.5361077859104439   T   T   T
  0.8325963388575106  0.1689437397413927  0.7021210273804612   T   T   T
  0.5000302576161886  0.5000245545708069  0.3790859498024091   F   F   F
  0.6666779694043186  0.8333199781470384  0.2933258797492897   F   F   F
  0.8333015827398924  0.6666722663589084  0.4648242920125725   F   F   F
  0.4964533863674832  0.5016180370038370  0.6208256236239172   T   T   T
  0.6685222893013824  0.8343523930787978  0.5350167300551903   T   T   T
  0.8345761630831875  0.6657458444427938  0.7027016464597118   T   T   T
  0.1666477117881300  0.3332954235762315  0.4388988662554425   F   F   F
  0.3333418362248537  0.1666477117881300  0.3192513055064197   F   F   F
  0.1652206488718372  0.3306228195868950  0.6818750803515280   T   T   T
  0.3323376289796945  0.1665247664954388  0.5609775239772896   T   T   T
  0.1666420087427483  0.8333199781470384  0.4388988662554425   F   F   F
  0.3333361331794720  0.6666722663589084  0.3192513055064197   F   F   F
  0.1669516721925702  0.8341789509969157  0.6792521132539890   T   T   T
  0.3333496935003128  0.6663729340166865  0.5613745614525854   T   T   T
  0.6666836724497003  0.3332954235762315  0.4388988662554425   F   F   F
  0.8333072857853026  0.1666477117881300  0.3192513055064197   F   F   F
  0.6656329322595437  0.3343027594045217  0.6795974186967971   T   T   T
  0.8343730383954294  0.1663499032351302  0.5611747417348106   T   T   T
  0.6666779694043186  0.8333199781470384  0.4388988662554425   F   F   F
  0.8333015827398924  0.6666722663589084  0.3192513055064197   F   F   F
  0.6709453103992092  0.8366268262235913  0.6817569509499097   T   T   T
  0.8339151636523834  0.6677732035751714  0.5609952258291631   T   T   T
```

Figure 2. CO_2 Chemisorption

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.3817703389725289  0.6179274454716692  0.7599331824591262   T   T   T
  0.2615904817771322  0.4466158907397483  0.7754572675170558   T   T   T
  0.5531835160914439  0.7377863958046065  0.7754610148248430   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.0010605013208931 -0.0010599888800452  0.6223855835721316   T   T   T
  0.1645603169135743  0.3281701125587458  0.5348077282572367   T   T   T
  0.3348585740732137  0.1610481882640599  0.7000675054803038   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.0195869871371356  0.5114347826323565  0.6194639987640757   T   T   T
  0.1643811720106272  0.8355673203736997  0.5349979309413462   T   T   T
  0.3252676596568784  0.6746947950755771  0.7140058453831042   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.4883492428793202 -0.0195012482372766  0.6194566736509537   T   T   T
  0.6667939521314541  0.3332252994618017  0.5371595329351515   T   T   T
  0.8302032025739549  0.1695818604859461  0.6990461439818139   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.4923069177435687  0.5078004321733930  0.6226310385110583   T   T   T
  0.6718220683733118  0.8354543931607005  0.5348135202688590   T   T   T
  0.8389972436903470  0.6650630857636329  0.7000484062603427   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1604590423267856  0.3210521487364595  0.6828576227348186   T   T   T
  0.3322807865710343  0.1661800988172893  0.5606671363912827   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1627492515173143  0.8373145140874750  0.6754130678178595   T   T   T
  0.3340559362831686  0.6659182879043494  0.5617576932027234   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6643617608967791  0.3355220884373572  0.6808567427748580   T   T   T
  0.8343382214186923  0.1656972289853111  0.5615156151628976   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6788815450663718  0.8393152617673559  0.6828793432363629   T   T   T
  0.8337748312884740  0.6677242016626006  0.5606706013608771   T   T   T
```

Table S4. Optimized Fractional Coordinates for the CO_2 Chemisorption Structures Shown in Figure 3.

Figure 3. (001)

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.3817703389725289  0.6179274454716692  0.7599331824591262   T   T   T
  0.2615904817771322  0.4466158907397483  0.7754572675170558   T   T   T
  0.5531835160914439  0.7377863958046065  0.7754610148248430   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.0010605013208931 -0.0010599888800452  0.6223855835721316   T   T   T
  0.1645603169135743  0.3281701125587458  0.5348077282572367   T   T   T
  0.3348585740732137  0.1610481882640599  0.7000675054803038   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.0195869871371356  0.5114347826323565  0.6194639987640757   T   T   T
  0.1643811720106272  0.8355673203736997  0.5349979309413462   T   T   T
  0.3252676596568784  0.6746947950755771  0.7140058453831042   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.4883492428793202 -0.0195012482372766  0.6194566736509537   T   T   T
  0.6667939521314541  0.3332252994618017  0.5371595329351515   T   T   T
  0.8302032025739549  0.1695818604859461  0.6990461439818139   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.4923069177435687  0.5078004321733930  0.6226310385110583   T   T   T
  0.6718220683733118  0.8354543931607005  0.5348135202688590   T   T   T
  0.8389972436903470  0.6650630857636329  0.7000484062603427   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1604590423267856  0.3210521487364595  0.6828576227348186   T   T   T
  0.3322807865710343  0.1661800988172893  0.5606671363912827   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1627492515173143  0.8373145140874750  0.6754130678178595   T   T   T
  0.3340559362831686  0.6659182879043494  0.5617576932027234   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6643617608967791  0.3355220884373572  0.6808567427748580   T   T   T
  0.8343382214186923  0.1656972289853111  0.5615156151628976   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6788815450663718  0.8393152617673559  0.6828793432363629   T   T   T
```

```
  0.8337748312884740  0.6677242016626006  0.5606706013608771   T   T   T
```

Figure 3. (011)-I

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.3226751769868818  0.2903890020256840  0.7180881079042000   T   T   T
  0.4640904496206570  0.2748154498025357  0.7398311349407958   T   T   T
  0.1747657618190402  0.2845770810271387  0.7396097471472276   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0238835536635721  0.0914321688636062  0.5611702570851266   T   T   T
  0.1339435283694820  0.5244369653073393  0.5973203481032294   T   T   T
  0.4118219579996321  0.6579156363493847  0.5215539001056231   T   T   T
  0.3292381292104271  0.3124957808058018  0.6659724749086172   T   T   T
  0.4405106927374448  0.7378854401626573  0.7040242803628235   T   T   T
  0.2229814318534344  0.9051705935564988  0.6398414825815336   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5197716236486883  0.0782004350446295  0.5613294572064561   T   T   T
  0.6249134352547699  0.5149199436363753  0.5942913506798665   T   T   T
  0.9175302162475955  0.6629377096212316  0.5221136890306890   T   T   T
  0.8162955947168308  0.2911143869916835  0.6625693989014220   T   T   T
  0.9349940410880515  0.7524319256005279  0.7081516549289392   T   T   T
  0.7257049494902822  0.8823116376400643  0.6364764545288631   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2056469330120352  0.8227656738879979  0.5504507947004816   T   T   T
  0.3364178697756174  0.3572120189831476  0.5665767119561365   T   T   T
 -0.0011748790817136  0.0481253998383193  0.6651640782210970   T   T   T
  0.1463777511045211  0.6037464979773338  0.6865206326368575   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7032197310151191  0.8159433172293384  0.5475984222906625   T   T   T
  0.8402909327842544  0.3549218286203165  0.5694890385145642   T   T   T
  0.5223297347152286  0.0378002380798411  0.6640096159235551   T   T   T
  0.6573040230401477  0.5845729671145145  0.6846477851049281   T   T   T
```

Figure 3. (011)-II

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.4029888504919800  0.6152604688030877  0.7590318870729269   T   T   T
  0.5336661004620662  0.5563775160988584  0.7731924089275540   T   T   T
  0.2429590097298212  0.5502203576509873  0.7727373944949834   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0222618613117094  0.0748295542441098  0.5653388385987771   T   T   T
  0.1272394263269802  0.5160956128421873  0.5932733415097425   T   T   T
  0.4175167604005103  0.6677408223690335  0.5213334440578803   T   T   T
  0.3233887927885615  0.2826256607291601  0.6618695572729940   T   T   T
  0.4347879323544974  0.7489275230636686  0.7197668266148231   T   T   T
  0.2318768904134485  0.8780648575188382  0.6391842901348990   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5224519661967268  0.0922454524957360  0.5655432760105922   T   T   T
  0.6314092573753227  0.5270356227382066  0.5941317511165345   T   T   T
  0.9145207411365548  0.6635332059433943  0.5216141055240979   T   T   T
  0.8260376627629463  0.3318740678319191  0.6665425511461367   T   T   T
  0.9432091588069454  0.7612431384441397  0.7040808163765302   T   T   T
  0.7155431348055703  0.8958364847192117  0.6400259260539137   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2040854064175425  0.8173109622836665  0.5489663593021822   T   T   T
  0.3417811668591196  0.3608453329801706  0.5691095068660120   T   T   T
  0.0209483694132366  0.0492108319574967  0.6605109637005583   T   T   T
  0.1259397398694916  0.5814227001396177  0.6851178538920829   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7053349438540357  0.8227392677266357  0.5498104260156323   T   T   T
  0.8367666133763474  0.3612715439197159  0.5690598611006304   T   T   T
  0.5097255195477255  0.0614303532769322  0.6617252464588255   T   T   T
  0.6673011781595717  0.5924484934824540  0.6855510370483567   T   T   T
```

Figure 3. (011)-III

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.3705750032534995  0.8296630698822141  0.7540773909162407   T   T   T
  0.4365330979827777  0.0088886067029683  0.7583421441492847   T   T   T
  0.2356521547164099  0.7254218281988712  0.7756836438436400   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0251113725156107  0.0765070513580789  0.5656555580886869   T   T   T
  0.1264157167617013  0.5176345750243360  0.5939640194172536   T   T   T
  0.4165387243670259  0.6637228822566565  0.5216763209597489   T   T   T
  0.3182137996136361  0.2957482882557331  0.6624869648087850   T   T   T
  0.4469090054048151  0.7439581931094120  0.7161417211599617   T   T   T
  0.2336683678659101  0.8783256959012689  0.6406122866765648   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5224392526139470  0.0913793429304675  0.5609943161813521   T   T   T
  0.6305697206548461  0.5241832139770692  0.5945132340263045   T   T   T
  0.9146555053234432  0.6636032543744816  0.5218086005873497   T   T   T
  0.8254325559756331  0.3256403319514342  0.6665434046535252   T   T   T
  0.9323340577634688  0.7438037334935734  0.7011361357053179   T   T   T
  0.7156533174391291  0.8938361353448734  0.6385645581619882   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2062129796485120  0.8176904518901008  0.5495824008441180   T   T   T
  0.3387136303823329  0.3564441382663182  0.5687871592350456   T   T   T
  0.0203185721727746  0.0405176172394689  0.6608946974614474   T   T   T
  0.1285271562711792  0.5727896321872953  0.6849516517782512   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7040423828591192  0.8232573067783062  0.5487150340206299   T   T   T
  0.8370845194855818  0.3590360120256398  0.5686125597721026   T   T   T
  0.5165841189417111  0.0664906797633611  0.6646995514573064   T   T   T
  0.6569435635630397  0.5891668607079807  0.6819609846400263   T   T   T
```

Figure 3. (100)

```
C O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.5095608658341177
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.8804724666706714  0.1648053120173406  0.7688159900528349   T   T   T
  0.8875746420279716 -0.0042384838895847  0.7959877364866739    T   T   T
  0.8825295488126205  0.3630483865986472  0.7815414282621903   T   T   T
  0.3750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.1250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.1250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.1250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.3750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.3750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.3751816197209042  0.5134093842790404  0.5567424969922566   T   T   T
  0.1345850231748127  0.1508920781994968  0.6064224947137734   T   T   T
  0.1218175433833078  0.8590135393525482  0.5212665191655294   T   T   T
  0.1239494060512824  0.5636396152858620  0.6891576355812504   T   T   T
  0.3742437093461120  0.0679867346779525  0.7281596160460884   T   T   T
  0.3759247594261880  0.8398614421815737  0.6436031135929177   T   T   T
  0.8750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.6250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.6250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.6250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.8750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.8750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.8753773334304217  0.4847971770972375  0.5634095852372714   T   T   T
  0.6170472506245172  0.1512043639116626  0.6064791997720050   T   T   T
  0.6283537999546388  0.8590203233364838  0.5213904381301269   T   T   T
  0.6282249956228287  0.5661448709189925  0.6897620871439597   T   T   T
  0.8697323614569782  0.1183379505510551  0.7209702143475964   T   T   T
  0.8762483353154870  0.8495102124125186  0.6419682206876028   T   T   T
  0.1250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.1250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.3750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.3750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.1276834874618652  0.7390438835052532  0.6027019356821030   T   T   T
  0.1274626385190794  0.2522685639729033  0.5206468775677898   T   T   T
  0.3757040014417269  0.7252363854900722  0.7230983749411017   T   T   T
  0.3755070517293734  0.2211475745434741  0.6553148991528969   T   T   T
  0.6250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.6250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.8750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.8750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.6243970052246486  0.7394870592908281  0.6028695012285197   T   T   T
  0.6226357096066744  0.2523310444126959  0.5207010723992485   T   T   T
  0.8770133110963062  0.7065415381019692  0.7259817596424232   T   T   T
  0.8758217459013573  0.2371562389864346  0.6406783669831576   T   T   T
```

Figure 3. (110)-I

```
C O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   C    O    La
     1    20    12
Selective dynamics
Direct
  0.5023653358528936  0.5031902944156695  0.7454900382226312   T   T   T
  0.6407590048704765  0.4015824718102929  0.7688847570328489   T   T   T
  0.3654863047107608  0.6071354629803363  0.7688985004272009   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.4999933582166168  0.5002781985095568  0.5374270983377752   T   T   T
  0.8352967932960350  0.8544303087355820  0.5397885932589125   T   T   T
  0.1649538662872714  0.1457311174573387  0.5398246985995223   T   T   T
  0.0000037286488979  0.4996928013076128  0.6230714229220877   T   T   T
  0.3327777789949120  0.8528415030347117  0.6190890088383270   T   T   T
  0.6669523772643701  0.1474644066856178  0.6189786643719534   T   T   T
  0.5005876418700735  0.5002395702339143  0.6902794168708938   T   T   T
  0.8369630371850333  0.8630038326855984  0.6968571441045056   T   T   T
  0.1632989954607872  0.1376951625869730  0.6970014010248754   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8306251460486898  0.2534494673555590  0.5387679683574524   T   T   T
  0.1695607680629813  0.7467515796338395  0.5387889814001868   T   T   T
  0.3260745472648185  0.2480664538468835  0.6198683659928441   T   T   T
  0.6739167095713380  0.7524923384471631  0.6197997572157441   T   T   T
  0.8390197546774655  0.2345067916442919  0.6971494681436919   T   T   T
  0.1612327803405601  0.7663115438791375  0.6973078003164442   T   T   T
```

Figure 3. (110)-II

```
C O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   C    O    La
     1    20    12
Selective dynamics
Direct
```

```
  0.8273737586664904  0.7888821257119988  0.7542864636686155   T   T   T
  0.9058074800302494  0.5984135666661935  0.7621952349014878   T   T   T
  0.7874402768625552  0.9315448816819828  0.7885881163948321   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.5099136914607987  0.5026727804089464  0.5391470991984079   T   T   T
  0.8349649227255925  0.8556129592218285  0.5388537536672454   T   T   T
  0.1634816505764038  0.1523533366751543  0.5391371853571081   T   T   T
  0.0159291920880745  0.5223891585863164  0.6266004619792690   T   T   T
  0.3382628761952653  0.8635160575072832  0.6152428527135103   T   T   T
  0.6840945306397250  0.1470403380269310  0.6242400719827623   T   T   T
  0.4719767217780092  0.5191913850681483  0.6795980132500125   T   T   T
  0.8060361439993599  0.8426176731365240  0.7019923447478301   T   T   T
  0.1356529243292014  0.1163757833130010  0.6943433976634534   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8306652683730055  0.2465514387441773  0.5397981364259877   T   T   T
  0.1665327127535330  0.7493595056127142  0.5382289366730137   T   T   T
  0.3316800749779622  0.2479518030074307  0.6219456491009859   T   T   T
  0.6617933045694119  0.7353582783043905  0.6171958878802195   T   T   T
  0.8336574264566911  0.2468991845467971  0.7048116325053181   T   T   T
  0.1901003704434156  0.7319082910965194  0.6926041658690210   T   T   T
```

Figure 3. (101)-I

```
C O  La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.0069371423432361  0.0381970014334295  0.7336256982111439   T   T   T
  0.8554288369291660  0.0624652188890311  0.7601653822038239   T   T   T
  0.1698365942290350  0.0463392085833687  0.7508693443988923   T   T   T
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.0864921130228210  0.4839256557096531  0.5636857793145453   T   T   T
  0.4403476494308582  0.1399833219135033  0.5487892096724151   T   T   T
```

```
  0.7411560939682478  0.3160805997457618  0.5618579576979789   T   T   T
  0.2973111746003185  0.1866908308856569  0.6506237824538936   T   T   T
  0.6155882354681707  0.3246990310050588  0.6778162173875431   T   T   T
  0.9940886664942855  0.0047046881345331  0.6837245477422298   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.0885518676898096  0.9776532524514203  0.5602338425332118   T   T   T
  0.4399026841700072  0.6439686008085964  0.5490864343710914   T   T   T
  0.7411272622795768  0.8175940004648176  0.5638266391039113   T   T   T
  0.3363171408249239  0.6626157488324791  0.6546929589155276   T   T   T
  0.6174558289472546  0.8699081626303465  0.6763109769358401   T   T   T
  0.8807057563749864  0.5340749019409128  0.6707050290608839   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7398252623532585  0.0659553735405114  0.5095415817741941   T   T   T
  0.4173467632743576  0.3960662820066110  0.6002830586519271   T   T   T
  0.9608162069220941  0.2681642596047351  0.6283138857106018   T   T   T
  0.4926707454419089  0.1193634948163018  0.7168683843798065   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7377845605323470  0.5684176004636674  0.5099077566627890   T   T   T
  0.4103606206027352  0.8999248908447092  0.6001682105800213   T   T   T
  0.9627426390243883  0.7580581092236772  0.6289380383331578   T   T   T
  0.5894073210691952  0.6018098515834970  0.7066598258295235   T   T   T
```

Figure 3. (101)-II

```
C O  La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   C    O    La
     1    26    16
Selective dynamics
Direct
  0.2195431823605118  0.2494935151853423  0.7180561792628342   T   T   T
  0.3537212592067617  0.2499877191224992  0.7501924704919684   T   T   T
  0.0476338566674366  0.2669653746344727  0.7307029046944508   T   T   T
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.0960261641657362  0.4834990461901231  0.5573459598338694   T   T   T
  0.4324236524283635  0.1374524737507301  0.5533302728759423   T   T   T
  0.7360226358751758  0.3136867153272592  0.5593878280619314   T   T   T
  0.2664038876090066  0.2292757539797506  0.6686220894548512   T   T   T
```

```
  0.6340212700391213  0.3230728251705089  0.6719146523489122   T   T   T
  0.9214053899141526  0.0040926596116246  0.6686751442942368   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.1005293250329435  0.9633521307009980  0.5568879014519668   T   T   T
  0.4434157670213491  0.6417721006222373  0.5506315999807853   T   T   T
  0.7336544410787077  0.8195070763776309  0.5616425367311259   T   T   T
  0.3287329855155265  0.6578431049963178  0.6536438044590666   T   T   T
  0.5666116386000569  0.8824884535769155  0.6875364098918513   T   T   T
  0.8402224794518768  0.5603939904651606  0.6613728292154699   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7380731770792153  0.0639233195906927  0.5093541094735702   T   T   T
  0.4188707199102549  0.3963870630005100  0.5992785791842887   T   T   T
  0.9413206706392078  0.2698316439417424  0.6306003085127133   T   T   T
  0.6778625378571025  0.0867073939423102  0.7212267797352820   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7397944351132942  0.5658825508510146  0.5089644134339388   T   T   T
  0.4191545106173882  0.8900585276354266  0.6014374159784752   T   T   T
  0.9804300581958493  0.7521857638143106  0.6222890773080997   T   T   T
  0.5764554603331146  0.6014258917675814  0.7073240782824496   T   T   T
```

Figure 3. (111)-I

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O    C
    12    20     1
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5478367964378639  0.5216639556027575  0.2663169609997603   T   T   T
  0.0961742746496543  0.6009545730350596  0.3496433071428779   T   T   T
  0.6775566802466968  0.7748734204686250  0.3998825436352105   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1106109662052538  0.9747429749842554  0.2250597083537680   T   T   T
  0.6518696051628035  0.0615680100389434  0.2918232629587286   T   T   T
  0.2907806839600374  0.1434496113748520  0.3828209813794672   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
```

```
  0.3621512622571447  0.7647979718201138  0.2413973566185627   T   T   T
  0.8037146622303358  0.8278505402046054  0.3106135223450648   T   T   T
  0.4371840629909373  0.9041542911007238  0.3658758737660274   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8435752256483171  0.0875435370362655  0.2142442637916543   T   T   T
  0.3573275740584206  0.1618498685117989  0.2941656614426914   T   T   T
  0.9220490783069598  0.2070017918775161  0.3842048670964185   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
  0.8583400539168128  0.4389936989423907  0.2758353967241529   T   T   T
  0.3804278654851773  0.4945005938413893  0.3602069417379085   T   T   T
  0.0243345570421415  0.8160082302576814  0.4053551912755420   T   T   T
  0.7061253446963635  0.3478436154680777  0.4086326660207010   T   T   T
  0.7155231631512283  0.0907996001951158  0.4569406502486171   T   T   T
  0.7782867899683928  0.2140217114414344  0.4188133410315141   T   T   T
```

Figure 3. (111)-II

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O    C
    12    20     1
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5503473366594361  0.5236306579780613  0.2665556404368335   T   T   T
  0.0924993015257324  0.5885381613804240  0.3402475343798669   T   T   T
  0.6124639522026600  0.6517559078197472  0.4241106019479955   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1041500631047435  0.9762499822500728  0.2254851117060768   T   T   T
  0.6617482473775330  0.0655780102190651  0.2978827542473657   T   T   T
  0.1548950673379499  0.1015028422034667  0.3679852929359979   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3433611960494438  0.7356183411938495  0.2526122589359465   T   T   T
  0.8718332914212629  0.8629078356147196  0.3037834574604921   T   T   T
  0.4425016667467201  0.9092945264694734  0.3862411182797128   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8294429790313885  0.0875229417802180  0.2155921296921929   T   T   T
  0.3616289063706762  0.1560051707952365  0.2934641523163447   T   T   T
  0.9288962794414045  0.2496951670414741  0.3620384435285764   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
```

```
  0.8420630879931396  0.4322903230580081  0.2723064227234736   T   T   T
  0.3966842791634841  0.4993294497254092  0.3569875775224871   T   T   T
  0.9450680138904924  0.7396073482927876  0.4049203026225520   T   T   T
  0.4719922032276620  0.1783868502578034  0.4351508678600707   T   T   T
  0.6074953790273999  0.9639343684674291  0.4639256036839989   T   T   T
  0.5108072890297526  0.0230779166450539  0.4300736352638407   T   T   T
```

Figure 3. (111)-III

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O    C
    12    20     1
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5671183210842501  0.5297639808230344  0.2604421725594651   T   T   T
 -0.0169796310323153  0.5134770174873723  0.3673385143665035   T   T   T
  0.5842370711999006  0.8121614008481204  0.4246460054075371   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1066971492640548  0.9854750319580988  0.2251489012163367   T   T   T
  0.6254275453829362  0.0374989673994218  0.2950029768786377   T   T   T
  0.1285176020240308  0.0450301313546545  0.3695013280475836   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3805998678457059  0.7535184492095679  0.2377750314184201   T   T   T
  0.8457625797456619  0.8492693468034799  0.2988210078407678   T   T   T
  0.3248997386756954  0.8249869561790560  0.3678874203703810   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8363241772882732  0.0980858153376439  0.2154613187846726   T   T   T
  0.3551757590830342  0.1787545396016354  0.2955263444208165   T   T   T
  0.8231620304324176  0.1362494669473102  0.3803454777751565   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
  0.8465919616188510  0.4210669544460213  0.2828466321716698   T   T   T
  0.3012703874429233  0.4381550503126122  0.4021563952674137   T   T   T
  0.8485895785164038  0.7204042630988499  0.4058313742237399   T   T   T
  0.3907463808635806  0.5209216390195111  0.4861504593294217   T   T   T
  0.2727826452108431  0.1906356954148674  0.4587340691571791   T   T   T
  0.3208634953103206  0.3787438287068612  0.4516914483207625   T   T   T
```

Table S5. Optimized Fractional Coordinates for the Stationary States Shown in Figure 5.

Figure 5 (a). O_2 Physisorption

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    26    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 -0.0009031953782231  0.0008441770181977  0.6204005201125846   T   T   T
  0.1670845165479568  0.3334108782167831  0.5349515971046188   T   T   T
  0.3338730478571227  0.1653793117573035  0.7043927244828531   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
 -0.0011368429562564  0.4971883806456222  0.6204377914782515   T   T   T
  0.1668454976192922  0.8331530992269213  0.5354792410546694   T   T   T
  0.3334894126133622  0.6665706195092375  0.7043969355302119   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.5027552791832446  0.0011557487914876  0.6205089045517403   T   T   T
  0.6665848372365164  0.3333359104970600  0.5350250683807192   T   T   T
  0.8341218971375665  0.1660891984302268  0.7052784688508045   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5001194755801527  0.4997388686074792  0.6202701053541078   T   T   T
  0.6665223081623416  0.8328829195526957  0.5349754397372405   T   T   T
  0.8347362546306130  0.6661626927344757  0.7043647069679605   T   T   T
  0.4184150454146157  0.4399828160892671  0.8174918237740508   T   T   T
  0.5709480890322227  0.6005692448310058  0.8177921000023148   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1668183890167258  0.3324345624086925  0.6808546106105240   T   T   T
  0.3337070165351256  0.1669887293443328  0.5611434402780449   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1673930067146234  0.8327140335374589  0.6805663045585595   T   T   T
  0.3337040849495069  0.6662767775263367  0.5611339085088058   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6679615070240671  0.3321222926044088  0.6804918257216783   T   T   T
  0.8334276426413308  0.1665223739371021  0.5611059790462781   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6677847189790167  0.8333554646853886  0.6808762775125788   T   T   T
  0.8329630949711503  0.6662837141507199  0.5611521501375959   T   T   T
```

Figure 5 (a). O_2 Transition State

```
O    La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095201    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999999
   O    La
    26    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
  0.0192440032893259  0.0030841266871954  0.6212007843285109   T   T   T
  0.1655042846689095  0.3374123631841708  0.5358193735041542   T   T   T
  0.3281908008213666  0.1502195244576970  0.7164773115732098   T   T   T
  0.9999922729179431  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.9889765945432869  0.5028385252538022  0.6218591788504227   T   T   T
  0.1686579040583493  0.8308531677009682  0.5352416284494677   T   T   T
  0.3274711824057294  0.6674883621606456  0.6977504322572479   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4863505205011039  0.0185995361583516  0.6219021429643659   T   T   T
  0.6713640096210703  0.3333016363082641  0.5338154744410895   T   T   T
  0.8344025870655747  0.1576677189937095  0.7042401740875240   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5164646048039118  0.4993278093399394  0.6189609731733055   T   T   T
  0.6661000319177599  0.8374038463969743  0.5363378519575726   T   T   T
  0.8601155667052018  0.6797258937768546  0.7103377185764957   T   T   T
  0.3451263820521475  0.2933501364624106  0.7551108872453525   T   T   T
  0.6142203671617505  0.5253664722482094  0.7376719544578598   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1647677428749513  0.3291590821249686  0.6847212919318189   T   T   T
  0.3366234948323021  0.1692302643575862  0.5610754465362077   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1698309655010368  0.8313679381267743  0.6748326282662057   T   T   T
  0.3348143200457158  0.6668003049615405  0.5609853456037746   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6798173163819992  0.3349233143032241  0.6807715577719228   T   T   T
  0.8350690359220813  0.1693112301446485  0.5616658862465445   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6607876454942493  0.8137663404352871  0.6874045175438170   T   T   T
  0.8315433828980534  0.6651700069782283  0.5608355089607904   T   T   T
```

Figure 5 (a). O_2 Chemisorption

```
O La C H
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
```

```
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    26    16
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.3790943669879780   F   F   F
  0.1666325478852855  0.3332650957705710  0.2933258797492897   F   F   F
  0.3333486385380624  0.1666325478852855  0.4648237441093741   F   F   F
 -0.0078255630831968  0.0109445326211028  0.6194731047828126   T   T   T
  0.1695683633978310  0.3361053222902954  0.5350088000124196   T   T   T
  0.2982634270600202  0.1209721781866457  0.7090329968211897   T   T   T
  0.9999897345183015  0.5000441982274353  0.3790943669879780   F   F   F
  0.1666222824035870  0.8333092939980062  0.2933258797492897   F   F   F
  0.3333383730563639  0.6666767461127208  0.4648237441093741   F   F   F
  0.0071724165316617  0.5064725949119965  0.6196752430695069   T   T   T
  0.1668125060567144  0.8336244718075376  0.5369399886917616   T   T   T
  0.3334098834491682  0.6703782430694607  0.6997404274999351   T   T   T
  0.4999378092088094  0.0000000000000000  0.3790943669879780   F   F   F
  0.6665703570940948  0.3332650957705710  0.2933258797492897   F   F   F
  0.8332864477468647  0.1666325478852855  0.4648237441093741   F   F   F
  0.4963236342230963 -0.0026218703431821  0.6200990762402502   T   T   T
  0.6676280265484529  0.3337382236035167  0.5338595863576125   T   T   T
  0.8260843079663664  0.1771944937008900  0.7075812562088925   T   T   T
  0.5000544637091338  0.5000441982274353  0.3790943669879780   F   F   F
  0.6666870115944192  0.8333092939980062  0.2933258797492897   F   F   F
  0.8332761822651662  0.6666767461127208  0.4648237441093741   F   F   F
  0.5142352626034233  0.4813324699320201  0.6239210664408793   T   T   T
  0.6646662799779239  0.8306576112916476  0.5353560741029467   T   T   T
  0.8792649639173440  0.7016075869607625  0.7079090421127373   T   T   T
  0.3728916335014817  0.2924673232683242  0.7434555181039718   T   T   T
  0.7102476440898402  0.6299661480633106  0.7431429515689285   T   T   T
  0.1666325478852855  0.3332650957705710  0.4388937363395371   F   F   F
  0.3333486385380624  0.1666325478852855  0.3192558875191267   F   F   F
  0.1561392588544647  0.3325477591663656  0.6842141158638556   T   T   T
  0.3380745216619270  0.1723391012298531  0.5611355371314001   T   T   T
  0.1666222824035870  0.8333092939980062  0.4388937363395371   F   F   F
  0.3333383730563639  0.6666767461127208  0.3192558875191267   F   F   F
  0.1793112090637834  0.8235562146922429  0.6681662770818688   T   T   T
  0.3338092761720997  0.6660985913798112  0.5594180806072888   T   T   T
  0.6665703570940948  0.3332650957705710  0.4388937363395371   F   F   F
  0.8332864477468647  0.1666325478852855  0.3192558875191267   F   F   F
  0.6513275009290018  0.3486997321957436  0.6916967907021034   T   T   T
  0.8340186934297500  0.1669227482621798  0.5629409286317358   T   T   T
  0.6666870115944192  0.8333092939980062  0.4388937363395371   F   F   F
  0.8332761822651662  0.6666767461127208  0.3192558875191267   F   F   F
  0.6710169600994945  0.8481592024078058  0.6844142983836748   T   T   T
  0.8289088856117421  0.6625566322110367  0.5610813481085781   T   T   T
```

Figure 5 (b). O_2 Physisorption on O_{5c}

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
```

```
   O    La
    26    16
Selective dynamics
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450857  0.4421844446604553   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
  0.1056635449218319  0.4226541796873349  0.4060585176142055   F   F   F
  0.0204297431280033  0.0843511925893536  0.5623608611836756   T   T   T
  0.1307121104342525  0.5232620377684090  0.5937312350252788   T   T   T
  0.4161228504779564  0.6621099385823097  0.5212234476900891   T   T   T
  0.3157092023111468  0.3010957999843178  0.6644503976522850   T   T   T
  0.4376750969437918  0.7538825219346793  0.7055888584375953   T   T   T
  0.2241605357542670  0.8909553949449971  0.6362488235332019   T   T   T
  0.9041292150553417  0.6166361650044720  0.3264885496827432   F   F   F
  0.5109466408572771  0.0440353265938924  0.3626144767290000   F   F   F
  0.7972975304409005  0.1893094265467212  0.2904013428155352   F   F   F
  0.7124330387450755  0.8499809181450857  0.4421844446604553   F   F   F
  0.8193151937378502  0.2773800797345061  0.4782716515276633   F   F   F
  0.6056013541306413  0.4226541796873349  0.4060585176142055   F   F   F
  0.5221432231763512  0.0868006565382146  0.5619175633385429   T   T   T
  0.6300336920956683  0.5211972573353300  0.5953341512642626   T   T   T
  0.9147803268188138  0.6624044166881528  0.5212362550273403   T   T   T
  0.8345400268684593  0.3024380886071584  0.6646527976904917   T   T   T
  0.9385265295262163  0.7543608205734935  0.7056305747090452   T   T   T
  0.7207654767294706  0.8920490515085605  0.6367650727898337   T   T   T
  0.5072579001561583  0.3329782479272146  0.7676003081482112   T   T   T
  0.5959888854181039  0.2127024110884745  0.7646523301283176   T   T   T
  0.0872918933927096  0.3491675735708455  0.3165761838479781   F   F   F
  0.2210261891095229  0.8841047564380986  0.3364396356965571   F   F   F
  0.3956958444457825  0.5826539194014728  0.4322333586466414   F   F   F
  0.0293804831775972  0.1175219327103818  0.4520968104952274   F   F   F
  0.2050911424695000  0.8203611952689104  0.5475343389834589   T   T   T
  0.3397105110776937  0.3572687673194784  0.5694033380738195   T   T   T
  0.0126950433062854  0.0511503268535527  0.6610728558948156   T   T   T
  0.1489046289450384  0.5978562994804479  0.6823712289246995   T   T   T
  0.5872297026015190  0.3491675735708455  0.3165761838479781   F   F   F
  0.7209639983183322  0.8841047564380986  0.3364396356965571   F   F   F
  0.8956336536545919  0.5826539194014728  0.4322333586466414   F   F   F
  0.5293182923863995  0.1175219327103818  0.4520968104952274   F   F   F
  0.7048032130486713  0.8202967393985948  0.5479345171178738   T   T   T
  0.8387155173393093  0.3573104003293638  0.5694749455730795   T   T   T
  0.5120602927936110  0.0493119298355902  0.6623663842301809   T   T   T
  0.6502125217344791  0.6012976460288962  0.6839985982322575   T   T   T
```

Figure 5 (b). O_2 Transition State on O_{5c}

```
O    La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995002    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284998
   O    La
    26    16
Selective dynamics
```

```
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450858  0.4421844446604551   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
  0.1056635449218320  0.4226541796873349  0.4060585176142055   F   F   F
  0.0182079837640052  0.0778767074237201  0.5605607014224296   T   T   T
  0.1253730715914692  0.5148610333069500  0.5943931665238938   T   T   T
  0.4148206766332640  0.6565141280380976  0.5223508963987056   T   T   T
  0.2927392393767271  0.3073037244096909  0.6658009400296132   T   T   T
  0.4320339106889686  0.7535503809466706  0.7082909152566402   T   T   T
  0.2185034252182426  0.8867672371554495  0.6362238323050616   T   T   T
  0.9041292150553417  0.6166361650044720  0.3264885496827432   F   F   F
  0.5109466408572771  0.0440353265938924  0.3626144767290000   F   F   F
  0.7972975304409076  0.1893094265467212  0.2904013428155352   F   F   F
  0.7124330387450755  0.8499809181450858  0.4421844446604551   F   F   F
  0.8193151937378502  0.2773800797345061  0.4782716515276633   F   F   F
  0.6056013541306413  0.4226541796873349  0.4060585176142055   F   F   F
  0.5185087955601831  0.0858028997096511  0.5581073788116820   T   T   T
  0.6270646444633587  0.5115676989730333  0.5990547961405674   T   T   T
  0.9093738938911352  0.6557025403569503  0.5220805601421554   T   T   T
  0.8679291272697203  0.3207381331372062  0.6675656988143541   T   T   T
  0.9402898375350807  0.7591058756236349  0.7081939734141345   T   T   T
  0.7203245117897579  0.8998276048435695  0.6376192076906256   T   T   T
  0.4901367250872691  0.2883305278371667  0.7302170057883463   T   T   T
  0.7117171738021313  0.2912493380792501  0.7176211414147989   T   T   T
  0.0872918933927096  0.3491675735708455  0.3165761838479781   F   F   F
  0.2210261891095229  0.8841047564380986  0.3364396356965571   F   F   F
  0.3956958444457825  0.5826539194014728  0.4322333586466413   F   F   F
  0.0293804831775972  0.1175219327103818  0.4520968104952272   F   F   F
  0.2021635315215952  0.8160642276440087  0.5476712918884045   T   T   T
  0.3386915969991859  0.3535333579578702  0.5684498789426153   T   T   T
  0.0094792368224179  0.0409184282241013  0.6628845822728698   T   T   T
  0.1475735951798907  0.5966559795495181  0.6845963547642872   T   T   T
  0.5872297026015190  0.3491675735708455  0.3165761838479781   F   F   F
  0.7209639983183322  0.8841047564380986  0.3364396356965571   F   F   F
  0.8956336536545919  0.5826539194014728  0.4322333586466413   F   F   F
  0.5293182923863995  0.1175219327103818  0.4520968104952272   F   F   F
  0.7022454935277439  0.8179508118234033  0.5499085976513752   T   T   T
  0.8341195662199548  0.3538271684810370  0.5676823584602629   T   T   T
  0.5020189502859262  0.0416115866831956  0.6662845453766741   T   T   T
  0.6466387945627678  0.5997763591324312  0.6894959280240757   T   T   T
```

Figure 5 (b). O_2 Chemisorption on O_{5c}

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    26    16
Selective dynamics
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
```

```
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450857  0.4421844446604553   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
  0.1056635449218319  0.4226541796873349  0.4060585176142055   F   F   F
  0.0216701582538979  0.0866904154167974  0.5586788837593853   T   T   T
  0.1292294714631477  0.5171796945954125  0.5958870148435529   T   T   T
  0.4143904708260573  0.6577135160177046  0.5220721554632297   T   T   T
  0.3273055123936119  0.3101338554737041  0.6626574150325110   T   T   T
  0.4351720189737956  0.7408860680002223  0.7081818494509560   T   T   T
  0.2220859556617760  0.8879691136550004  0.6392962634224850   T   T   T
  0.9041292150553417  0.6166361650044720  0.3264885496827432   F   F   F
  0.5109466408572771  0.0440353265938924  0.3626144767290000   F   F   F
  0.7972975304409005  0.1893094265467212  0.2904013428155352   F   F   F
  0.7124330387450755  0.8499809181450857  0.4421844446604553   F   F   F
  0.8193151937378502  0.2773800797345061  0.4782716515276633   F   F   F
  0.6056013541306413  0.4226541796873349  0.4060585176142055   F   F   F
  0.5216554459925576  0.0866885428291218  0.5586488058960819   T   T   T
  0.6291924309557253  0.5171969446011617  0.5958730698661487   T   T   T
  0.9143806206890044  0.6577694149147929  0.5220678750933627   T   T   T
  0.8270755999047666  0.3101068769591326  0.6626148527864126   T   T   T
  0.9352111742877968  0.7408609892372532  0.7081300196723698   T   T   T
  0.7219057107852075  0.8879664491215213  0.6392935216958819   T   T   T
  0.3046100381265324  0.2188436332725363  0.7147283767364226   T   T   T
  0.8050214499002257  0.2189319126895427  0.7147101756186235   T   T   T
  0.0872918933927096  0.3491675735708455  0.3165761838479781   F   F   F
  0.2210261891095229  0.8841047564380986  0.3364396356965571   F   F   F
  0.3956958444457825  0.5826539194014728  0.4322333586466414   F   F   F
  0.0293804831775972  0.1175219327103818  0.4520968104952274   F   F   F
  0.2044434310658280  0.8178911837292113  0.5496884935357594   T   T   T
  0.3376085167243421  0.3507112665329211  0.5668626413263159   T   T   T
  0.0103696526204827  0.0414699914591311  0.6700135810961527   T   T   T
  0.1484070315641470  0.5936101330859326  0.6848416075465475   T   T   T
  0.5872297026015190  0.3491675735708455  0.3165761838479781   F   F   F
  0.7209639983183322  0.8841047564380986  0.3364396356965571   F   F   F
  0.8956336536545919  0.5826539194014728  0.4322333586466414   F   F   F
  0.5293182923863995  0.1175219327103818  0.4520968104952274   F   F   F
  0.7044113642198164  0.8179470857190397  0.5496733092536928   T   T   T
  0.8376057580395403  0.3507593578093860  0.5668625171674749   T   T   T
  0.5103383761123014  0.0415175838560166  0.6700584509759169   T   T   T
  0.6483664092532817  0.5937024306134786  0.6848217620053577   T   T   T
```

Figure 5 (b). O_2 Physisorption on O_{5c}/O_{3c}

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    26    16
Selective dynamics
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450857  0.4421844446604553   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
```

```
  0.1056635449218319  0.4226541796873349  0.4060585176142055   F   F   F
  0.0209480597829943  0.0841545417415301  0.5626525767925787   T   T   T
  0.1300535117766939  0.5205876633308703  0.5945927457457483   T   T   T
  0.4153363980599523  0.6614202087742724  0.5213234296923406   T   T   T
  0.3241739559017327  0.2971361751004384  0.6652328800606530   T   T   T
  0.4380842504294893  0.7522139667669966  0.7061159667785147   T   T   T
  0.2218695457793743  0.8881407131054757  0.6364821510385892   T   T   T
  0.9041292150553417  0.6166361650044720  0.3264885496827432   F   F   F
  0.5109466408572771  0.0440353265938924  0.3626144767290000   F   F   F
  0.7972975304409076  0.1893094265467212  0.2904013428155352   F   F   F
  0.7124330387450755  0.8499809181450857  0.4421844446604553   F   F   F
  0.8193151937378502  0.2773800797345061  0.4782716515276633   F   F   F
  0.6056013541306413  0.4226541796873349  0.4060585176142055   F   F   F
  0.5210759243440800  0.0840367264219515  0.5626551198738607   T   T   T
  0.6301011403932379  0.5202964755767083  0.5945908025373137   T   T   T
  0.9153880652642333  0.6615536612969003  0.5213084854058425   T   T   T
  0.8239386283100748  0.2954971023993897  0.6653433174662532   T   T   T
  0.9377352694847759  0.7514405574749300  0.7062638074101207   T   T   T
  0.7219733190009684  0.8875649561399337  0.6364351632590638   T   T   T
  0.3592861168860335  0.3542110473384208  0.8056481125471507   T   T   T
  0.4007033417340247  0.4911964414674803  0.8354916038510034   T   T   T
  0.0872918933927096  0.3491675735708455  0.3165761838479781   F   F   F
  0.2210261891095229  0.8841047564380986  0.3364396356965571   F   F   F
  0.3956958444457825  0.5826539194014728  0.4322333586466414   F   F   F
  0.0293804831775972  0.1175219327103818  0.4520968104952274   F   F   F
  0.2046348805971054  0.8187392974033481  0.5478107593013642   T   T   T
  0.3389073606930887  0.3558100424341329  0.5696967195551753   T   T   T
  0.0119450944397564  0.0493083659735797  0.6612671530664462   T   T   T
  0.1496499448157536  0.5982641339778952  0.6830266356258636   T   T   T
  0.5872297026015190  0.3491675735708455  0.3165761838479781   F   F   F
  0.7209639983183322  0.8841047564380986  0.3364396356965571   F   F   F
  0.8956336536545919  0.5826539194014728  0.4322333586466414   F   F   F
  0.5293182923863995  0.1175219327103818  0.4520968104952274   F   F   F
  0.7046484681793334  0.8186619521044066  0.5477846736992478   T   T   T
  0.8389544019094359  0.3557800439984105  0.5697039123262614   T   T   T
  0.5126765471285102  0.0494762653409311  0.6612135577006734   T   T   T
  0.6492388444047472  0.5978857029480258  0.6830558522323776   T   T   T
```

Figure 5 (b). O_2 Transition State on O_{5c}/O_{3c}

```
O    La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995002    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284998
   O    La
    26    16
Selective dynamics
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450858  0.4421844446604551   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
  0.1056635449218320  0.4226541796873349  0.4060585176142055   F   F   F
  0.0223165726904202  0.0857859285055644  0.5622201437221732   T   T   T
  0.1330430285029629  0.5206153378177351  0.5964629817852368   T   T   T
```

```
  0.4142701969463777  0.6591018891541892  0.5213878396423378   T   T   T
  0.3198619533481042  0.2844903370766440  0.6587706112514997   T   T   T
  0.4507822467657283  0.7833699849280675  0.7128349028306241   T   T   T
  0.2236780532713367  0.8914292347052963  0.6388209222524580   T   T   T
  0.9041292150553417  0.6166361650044720  0.3264885496827432   F   F   F
  0.5109466408572771  0.0440353265938924  0.3626144767290000   F   F   F
  0.7972975304409076  0.1893094265467212  0.2904013428155352   F   F   F
  0.7124330387450755  0.8499809181450858  0.4421844446604551   F   F   F
  0.8193151937378502  0.2773800797345061  0.4782716515276633   F   F   F
  0.6056013541306413  0.4226541796873349  0.4060585176142055   F   F   F
  0.5216349379620241  0.0837745908696213  0.5615366987426177   T   T   T
  0.6264389882056118  0.5181649582098004  0.5954499564269783   T   T   T
  0.9158770236011028  0.6611869887591107  0.5221756643737219   T   T   T
  0.8194030322093677  0.2944356521703580  0.6665379870066884   T   T   T
  0.9379146772085111  0.7576059512399329  0.7090679005375555   T   T   T
  0.7226342921120651  0.8873164658241147  0.6375021007287405   T   T   T
  0.3139382039532883  0.2552074457560927  0.7143242016726882   T   T   T
  0.3786170205553075  0.5065746656613168  0.7316723087161723   T   T   T
  0.0872918933927096  0.3491675735708455  0.3165761838479781   F   F   F
  0.2210261891095229  0.8841047564380986  0.3364396356965571   F   F   F
  0.3956958444457825  0.5826539194014728  0.4322333586466413   F   F   F
  0.0293804831775972  0.1175219327103818  0.4520968104952272   F   F   F
  0.2050057221462847  0.8194228796667815  0.5499388095971219   T   T   T
  0.3382196918733193  0.3564815027164018  0.5663444188059971   T   T   T
  0.0061527734759855  0.0473761990080682  0.6643935583146403   T   T   T
  0.1523122972366753  0.6078223065461804  0.6867272185845640   T   T   T
  0.5872297026015190  0.3491675735708455  0.3165761838479781   F   F   F
  0.7209639983183322  0.8841047564380986  0.3364396356965571   F   F   F
  0.8956336536545919  0.5826539194014728  0.4322333586466413   F   F   F
  0.5293182923863995  0.1175219327103818  0.4520968104952272   F   F   F
  0.7043595590596150  0.8176389823247839  0.5484178445853581   T   T   T
  0.8399405192651703  0.3569020522049509  0.5701521181856554   T   T   T
  0.5212261128406880  0.0534993367367090  0.6639748976809111   T   T   T
  0.6535390370186910  0.5992108355800939  0.6860923248482834   T   T   T
```

Figure 5 (b). O_2 Chemisorption on O_{5c}/O_{3c}

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    26    16
Selective dynamics
Direct
  0.4041914058465323  0.6166361650044720  0.3264885496827432   F   F   F
  0.0110088316484749  0.0440353265938924  0.3626144767290000   F   F   F
  0.2973597212320982  0.1893094265467212  0.2904013428155352   F   F   F
  0.2124952295362732  0.8499809181450857  0.4421844446604553   F   F   F
  0.3193773845290409  0.2773800797345061  0.4782716515276633   F   F   F
  0.1056635449218319  0.4226541796873349  0.4060585176142055   F   F   F
  0.0239454619378810  0.0782921025258686  0.5615633552100852   T   T   T
  0.1274247048782464  0.5128284513626185  0.5980752894017156   T   T   T
  0.4102101533620168  0.6585367274395943  0.5212923130789758   T   T   T
  0.3432053531699767  0.3193004352805056  0.6654381747463863   T   T   T
  0.4571681408352712  0.7937369506310304  0.7161360850251867   T   T   T
```

0.2317372871624053	0.8902771055794463	0.6378628887253844	T	T	T
0.9041292150553417	0.6166361650044720	0.3264885496827432	F	F	F
0.5109466408572771	0.0440353265938924	0.3626144767290000	F	F	F
0.7972975304409005	0.1893094265467212	0.2904013428155352	F	F	F
0.7124330387450755	0.8499809181450857	0.4421844446604553	F	F	F
0.8193151937378502	0.2773800797345061	0.4782716515276633	F	F	F
0.6056013541306413	0.4226541796873349	0.4060585176142055	F	F	F
0.5239974964960656	0.0838868785515826	0.5620953185545750	T	T	T
0.6206071385286926	0.5174087491927513	0.5942220996697908	T	T	T
0.9136697744020795	0.6584517544755971	0.5224672276086785	T	T	T
0.7889648261122005	0.3049652404376947	0.6655936089941746	T	T	T
0.9422981323444038	0.7417114707796959	0.7062977389058342	T	T	T
0.7190568354102990	0.8835446439084409	0.6371539031539367	T	T	T
0.2150690525484313	0.2712410068399548	0.7092389564357272	T	T	T
0.4191885253453577	0.6153345972611493	0.7456912438132132	T	T	T
0.0872918933927096	0.3491675735708455	0.3165761838479781	F	F	F
0.2210261891095229	0.8841047564380986	0.3364396356965571	F	F	F
0.3956958444457825	0.5826539194014728	0.4322333586466414	F	F	F
0.0293804831775972	0.1175219327103818	0.4520968104952274	F	F	F
0.2021967738908775	0.8163797481999890	0.5498114870224268	T	T	T
0.3341539864852250	0.3568710046754712	0.5668661317524784	T	T	T
0.0115528014910052	0.0336294906384354	0.6613181431807851	T	T	T
0.1614771768364434	0.5932167311845880	0.6895813054189165	T	T	T
0.5872297026015190	0.3491675735708455	0.3165761838479781	F	F	F
0.7209639983183322	0.8841047564380986	0.3364396356965571	F	F	F
0.8956336536545919	0.5826539194014728	0.4322333586466414	F	F	F
0.5293182923863995	0.1175219327103818	0.4520968104952274	F	F	F
0.7014177639827680	0.8161846787302721	0.5481174348280616	T	T	T
0.8355393130017600	0.3579126003688162	0.5703886539067933	T	T	T
0.5234448848174835	0.0562814074082417	0.6612589340822538	T	T	T
0.6564898731539248	0.5900495951174078	0.6860953661540069	T	T	T

Table S6. Optimized Fractional Coordinates for the O_2 Chemisorption States Shown in Figure 6.

Figure 6. (001)

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -3.9394900000000002    6.8233968359095165    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.5688315207999963
   O    La
    25    16
Selective dynamics
Direct
  0.4141692187218539  0.3283385295773833  0.7396739790751481   T   T   T
  0.0000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.3333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.0024907849388112  0.0037696784797863  0.6194766682073491   T   T   T
  0.1653120435734066  0.3350594013180238  0.5348236247697372   T   T   T
  0.3197036893272461  0.1394081266114968  0.7113863593353295   T   T   T
  0.0000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.1666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.3333333333333357  0.6666666666666714  0.4648249768915562   F   F   F
  0.0035456896523880  0.5070949244064072  0.6228159884886313   T   T   T
  0.1651960058950865  0.8303921922811286  0.5355552048415761   T   T   T
  0.3361218621303447  0.6751619024971566  0.7026609786321270   T   T   T
  0.5000000000000000  0.0000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.3333333333333286  0.2933258797492897   F   F   F
  0.8333333333333286  0.1666666666666714  0.4648249768915562   F   F   F
  0.5012782132215111  0.0037710483354451  0.6194763926345923   T   T   T
  0.6697464072490040  0.3350591561511766  0.5348234289204110   T   T   T
  0.8353746640426996  0.1707502092782166  0.7055209188114961   T   T   T
  0.5000000000000000  0.5000000000000000  0.3790754283204265   F   F   F
  0.6666666666666714  0.8333333333333357  0.2933258797492897   F   F   F
  0.8333333333333286  0.6666666666666714  0.4648249768915562   F   F   F
  0.4899789892477361  0.4799578837479528  0.6207897859220195   T   T   T
  0.6660136788855295  0.8320283644762223  0.5355238312074382   T   T   T
  0.8390389430451122  0.6751619319617593  0.7026614962217229   T   T   T
  0.1666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.3333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.1717482302115272  0.3403148383034688  0.6828668342254185   T   T   T
  0.3343839940905268  0.1687681566889489  0.5612782885711838   T   T   T
  0.1666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.3333333333333357  0.6666666666666714  0.3192455779905217   F   F   F
  0.1602836202263209  0.8205691085362967  0.6757445607861525   T   T   T
  0.3337820655613621  0.6662553603057546  0.5606813490330671   T   T   T
  0.6666666666666714  0.3333333333333286  0.4389052786503242   F   F   F
  0.8333333333333286  0.1666666666666714  0.3192455779905217   F   F   F
  0.6685663220220242  0.3403150407923305  0.6828667734271688   T   T   T
  0.8327163596865769  0.1654337574377546  0.5618516015039017   T   T   T
  0.6666666666666714  0.8333333333333357  0.4389052786503242   F   F   F
  0.8333333333333286  0.6666666666666714  0.3192455779905217   F   F   F
  0.6700867818264707  0.8401738655807260  0.6828005158505046   T   T   T
  0.8324724427964884  0.6662551081806780  0.5606812684118307   T   T   T
```

Figure 6. (011)-I

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    25    16
Selective dynamics
Direct
  0.2250311841715522  0.2898079831338705  0.7138847842176839   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0243079952158200  0.0872813174718687  0.5603754691659287   T   T   T
  0.1287273203215221  0.5171492446570057  0.5969751411957614   T   T   T
  0.4106940941847147  0.6572720264183307  0.5214061867662593   T   T   T
  0.3422074361081899  0.3209670371743377  0.6669413423554355   T   T   T
  0.4460961204647600  0.7544676205771162  0.7067942113509592   T   T   T
  0.2256899772460379  0.8977938585196090  0.6373240913282694   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5226758723172047  0.0790686659450783  0.5610798160300280   T   T   T
  0.6225991720658060  0.5149639699890812  0.5942709298548735   T   T   T
  0.9146168958551666  0.6597749891485140  0.5220246528302941   T   T   T
  0.8012058868968708  0.2924031194457339  0.6650592955758914   T   T   T
  0.9397398260558411  0.7502245921202769  0.7072021062581665   T   T   T
  0.7250295167483655  0.8833951008357426  0.6361462484753997   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2028414843050396  0.8190069041191199  0.5493086548527446   T   T   T
  0.3337489077545140  0.3555218625187579  0.5669820386629173   T   T   T
  0.0112313305148585  0.0460631214008752  0.6638567109117063   T   T   T
  0.1565392177067624  0.5984114916202340  0.6864092944402802   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7023714856382136  0.8158615442761334  0.5474859213759630   T   T   T
  0.8366099633725815  0.3532916327663594  0.5700288057125457   T   T   T
  0.5205956830494373  0.0431147960930632  0.6620999122512381   T   T   T
  0.6553316506530105  0.5940859042281182  0.6835018999311384   T   T   T
```

Figure 6. (011)-II

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
```

```
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    25    16
Selective dynamics
Direct
  0.3054739409177753  0.2167533485744702  0.7130727935832181   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0229565800731640  0.0869865317668215  0.5610258432401687   T   T   T
  0.1311554893331585  0.5196389841786864  0.5950476035258861   T   T   T
  0.4151930726480768  0.6592686686425638  0.5212585521257689   T   T   T
  0.3279668873750614  0.3108486143737427  0.6614565997260150   T   T   T
  0.4363727162686686  0.7445028624016744  0.7059752882476296   T   T   T
  0.2208873971836291  0.8899895873171763  0.6368606350944872   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5198508813573394  0.0847097840146259  0.5611833495725685   T   T   T
  0.6284866547830739  0.5190942747162444  0.5949027109966359   T   T   T
  0.9147436021908267  0.6606871842790623  0.5217163963105194   T   T   T
  0.8240572697253289  0.2986030187333392  0.6663178145586309   T   T   T
  0.9369095155352243  0.7491991515262620  0.7073264098546754   T   T   T
  0.7232235698328527  0.8871295809028795  0.6379835954848336   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2041927986000861  0.8187148169115198  0.5481930887237407   T   T   T
  0.3383457573648394  0.3543548542822199  0.5665935520187072   T   T   T
  0.0121019437030124  0.0475582324401294  0.6647803830992132   T   T   T
  0.1467381375875399  0.5979061050660390  0.6836834484770455   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7050102583329773  0.8183416698247348  0.5485715779279104   T   T   T
  0.8383858638026260  0.3529015756009751  0.5701051918392327   T   T   T
  0.5103843567357083  0.0438742180757489  0.6645045598697743   T   T   T
  0.6514719506571399  0.5944906227736406  0.6836307058684099   T   T   T
```

Figure 6. (011)-III

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    25    16
```

```
Selective dynamics
Direct
  0.3054739409177753  0.2167533485744702  0.7130727935832181   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0229565800731640  0.0869865317668215  0.5610258432401687   T   T   T
  0.1311554893331585  0.5196389841786864  0.5950476035258861   T   T   T
  0.4151930726480768  0.6592686686425638  0.5212585521257689   T   T   T
  0.3279668873750614  0.3108486143737427  0.6614565997260150   T   T   T
  0.4363727162686686  0.7445028624016744  0.7059752882476296   T   T   T
  0.2208873971836291  0.8899895873171763  0.6368606350944872   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5198508813573394  0.0847097840146259  0.5611833495725685   T   T   T
  0.6284866547830739  0.5190942747162444  0.5949027109966359   T   T   T
  0.9147436021908267  0.6606871842790623  0.5217163963105194   T   T   T
  0.8240572697253289  0.2986030187333392  0.6663178145586309   T   T   T
  0.9369095155352243  0.7491991515262620  0.7073264098546754   T   T   T
  0.7232235698328527  0.8871295809028795  0.6379835954848336   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2041927986000861  0.8187148169115198  0.5481930887237407   T   T   T
  0.3383457573648394  0.3543548542822199  0.5665935520187072   T   T   T
  0.0121019437030124  0.0475582324401294  0.6647803830992132   T   T   T
  0.1467381375875399  0.5979061050660390  0.6836834484770455   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7050102583329773  0.8183416698247348  0.5485715779279104   T   T   T
  0.8383858638026260  0.3529015756009751  0.5701051918392327   T   T   T
  0.5103843567357083  0.0438742180757489  0.6645045598697743   T   T   T
  0.6514719506571399  0.5944906227736406  0.6836307058684099   T   T   T
```

Figure 6. (011)-IV

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
    -1.9697450000000001    7.0625114891995047    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.8263268595284643
   O    La
    25    16
Selective dynamics
Direct
  0.3470656159174417  0.8533390290720843  0.7375627643216904   T   T   T
  0.4041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
```

```
  0.0110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.2973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.2125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.3193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.1056615246639652  0.4226460986558749  0.4060669543983195   F   F   F
  0.0221391414328926  0.0821896402480144  0.5638541052649665   T   T   T
  0.1273915307930371  0.5153652069979264  0.5956852320078964   T   T   T
  0.4152910029044437  0.6612186939650723  0.5213360455610627   T   T   T
  0.3309023955495780  0.2896110059233085  0.6644571279923494   T   T   T
  0.4504919845203785  0.7364360944919551  0.7124850437160825   T   T   T
  0.2240316476536262  0.8824227482396355  0.6355577316913723   T   T   T
  0.9041697660885788  0.6166790643543223  0.3265015826258235   F   F   F
  0.5110175396903500  0.0440701587614001  0.3626018224361118   F   F   F
  0.7973219924868076  0.1892879699472374  0.2904013428155352   F   F   F
  0.7125092982657435  0.8500371930629598  0.4421671942086078   F   F   F
  0.8193570718675147  0.2774282874700376  0.4782674340188962   F   F   F
  0.6056615246639723  0.4226460986558749  0.4060669543983195   F   F   F
  0.5215597289639383  0.0891754302124535  0.5607787331919165   T   T   T
  0.6310650528138400  0.5253033351980414  0.5934524937593043   T   T   T
  0.9147456815392141  0.6616631848533080  0.5214498735234759   T   T   T
  0.8116656878831569  0.3251682911335977  0.6679089941620883   T   T   T
  0.9371151825643361  0.7547596934782576  0.7043422790111716   T   T   T
  0.7222102289763218  0.8951584868349627  0.6373752362535490   T   T   T
  0.0873093305305090  0.3492373221220291  0.3165603160863029   F   F   F
  0.2210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.3956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.0293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.2049096218184346  0.8158968486145152  0.5474160217753246   T   T   T
  0.3397707598594114  0.3547147954727447  0.5692084558346501   T   T   T
  0.0177482694389121  0.0464463705834047  0.6601358867676758   T   T   T
  0.1434579034204273  0.5993166389531633  0.6850552689644099   T   T   T
  0.5873093305305019  0.3492373221220291  0.3165603160863029   F   F   F
  0.7210302016466557  0.8841208065866084  0.3364428491653442   F   F   F
  0.8956488627076666  0.5825954508306666  0.4322259276690872   F   F   F
  0.5293697338238132  0.1174789352952530  0.4521084607481285   F   F   F
  0.7040188393124575  0.8231369386717150  0.5481740401716343   T   T   T
  0.8367618746873904  0.3565615144500894  0.5692833749438220   T   T   T
  0.5070023756402149  0.0518927738868904  0.6653210532441476   T   T   T
  0.6606429732372523  0.5861094327060971  0.6811416712246195   T   T   T
```

Figure 6. (100)-I

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.5095608658341177
   O    La
    25    16
Selective dynamics
Direct
  0.3750000000000000  0.2918565831222069  0.7411547560219336   T   T   T
  0.3750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.1250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.1250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.1250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.3750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
```

```
  0.3750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.3750000000000000  0.5125573012446264  0.5574951721448400   T   T   T
  0.1311423095097144  0.1507742739362595  0.6076321616308622   T   T   T
  0.1241582042655954  0.8617348935234332  0.5207319379209205   T   T   T
  0.1170419136437306  0.5621752986852013  0.6856374847683665   T   T   T
  0.3750000000000000  0.0561412508033619  0.7357491430241793   T   T   T
  0.3750000000000000  0.8308576484254416  0.6449492791850321   T   T   T
  0.8750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.6250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.6250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.6250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.8750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.8750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.8750000000000000  0.5036736549909400  0.5591105783916823   T   T   T
  0.6188576904902854  0.1507742739362595  0.6076321616308622   T   T   T
  0.6258417957344045  0.8617348935234332  0.5207319379209205   T   T   T
  0.6329580863562692  0.5621752986852013  0.6856374847683665   T   T   T
  0.8750000000000000  0.0818927433341074  0.7246195401655090   T   T   T
  0.8750000000000000  0.8490622352189531  0.6395972643354564   T   T   T
  0.1250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.1250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.3750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.3750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.1257164051010977  0.7331067308949040  0.6007613370184910   T   T   T
  0.1252894455123432  0.2511611257056939  0.5211753381222455   T   T   T
  0.3750000000000000  0.6730765509440679  0.7204352700487180   T   T   T
  0.3750000000000000  0.2065643406541682  0.6533817904390280   T   T   T
  0.6250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.6250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.8750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.8750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.6242835948989021  0.7331067308949040  0.6007613370184910   T   T   T
  0.6247105544876568  0.2511611257056939  0.5211753381222455   T   T   T
  0.8750000000000000  0.7387071766530082  0.7185525038521173   T   T   T
  0.8750000000000000  0.2305813887933597  0.6507358835219251   T   T   T
```

Figure 6. (100)-II

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.5095608658341177
   O    La
    25    16
Selective dynamics
Direct
  0.1249996664920867  0.5432356085623099  0.7453546221463226   T   T   T
  0.3750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.1250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.1250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.1250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.3750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.3750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.3746228898523965  0.5120810768463727  0.5569412907637326   T   T   T
  0.1249997001237652  0.1553750931808907  0.6086420319490604   T   T   T
  0.1249999400149668  0.8647336006275800  0.5215751140204630   T   T   T
```

```
  0.1249995440744254  0.5151721623786488  0.6908978233972338   T   T   T
  0.3912018998780488  0.0656090453069013  0.7276847184760872   T   T   T
  0.3700509036128277  0.8302017529007280  0.6427932502788805   T   T   T
  0.8750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.6250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.6250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.6250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.8750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.8750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.8753763738998370  0.5120811327541894  0.5569413012478499   T   T   T
  0.6249995755064062  0.1413297890522753  0.6077221187693703   T   T   T
  0.6250000403990474  0.8607127552024366  0.5210228621096575   T   T   T
  0.6249999837278331  0.5413428487828433  0.6870358001947674   T   T   T
  0.8587977918549039  0.0656091154510754  0.7276847910023440   T   T   T
  0.8799487406698120  0.8302018740384505  0.6427932303025733   T   T   T
  0.1250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.1250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.3750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.3750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.1249995757599779  0.7380120322064738  0.5991132120756387   T   T   T
  0.1250001976677288  0.2541814426823900  0.5217403969958119   T   T   T
  0.3843535776603231  0.7235375002823415  0.7230176003486352   T   T   T
  0.3794461766001302  0.2144587818799117  0.6544299681347735   T   T   T
  0.6250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.6250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.8750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.8750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.6249997592283111  0.7297036343064663  0.6011488495221663   T   T   T
  0.6250000625446632  0.2492251260942012  0.5213354789139740   T   T   T
  0.8656461961449348  0.7235374793414576  0.7230177559858751   T   T   T
  0.8705530704863752  0.2144590748528742  0.6544300246480366   T   T   T
```

Figure 6. (100)-III

```
O La
   1.00000000000000
     7.8789800000000003    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   27.5095608658341177
   O    La
    25    16
Selective dynamics
Direct
  0.3712839228368057 -0.0159347665440964  0.7754699669231729   T   T   T
  0.3750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
  0.1250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.1250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.1250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.3750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.3750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.3749911239907393  0.4985570360817034  0.5609626173383649   T   T   T
  0.1246332992092210  0.1517339930511841  0.6073026888138541   T   T   T
  0.1264629207571501  0.8603472280766735  0.5209172447808766   T   T   T
  0.1232032641325329  0.5543784683278280  0.6872430038342437   T   T   T
  0.3736878823449279  0.0960291583180095  0.7282113562866501   T   T   T
  0.3751039442407691  0.8458358311118573  0.6413532486640855   T   T   T
  0.8750000000000000  0.5000000000000000  0.3139720349630153   F   F   F
```

```
  0.6250000000000000  0.1454420000000027  0.3553115827490103   F   F   F
  0.6250000000000000  0.8545579999999973  0.2726324871770203   F   F   F
  0.6250000000000000  0.5000000000000000  0.4379906783210075   F   F   F
  0.8750000000000000  0.1454420000000027  0.4793302261070025   F   F   F
  0.8750000000000000  0.8545579999999973  0.3966511305350124   F   F   F
  0.8750183245226536  0.5103495231933859  0.5574279111176420   T   T   T
  0.6253959207778961  0.1518127678154950  0.6073286995977467   T   T   T
  0.6235452608322753  0.8603536008874859  0.5209465644221659   T   T   T
  0.6272349243836508  0.5546485338534677  0.6873660194464624   T   T   T
  0.8742719131922148  0.0694928185474641  0.7263084529444048   T   T   T
  0.8751495497844997  0.8406411626863725  0.6415200973921333   T   T   T
  0.1250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.1250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.3750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.3750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.1239425608695767  0.7334102380172243  0.6011024064138250   T   T   T
  0.1244991448609503  0.2511223096577951  0.5211630606687452   T   T   T
  0.3748118119964745  0.7139025986031567  0.7202534204890327   T   T   T
  0.3748441100854890  0.2232964359104871  0.6488459248427946   T   T   T
  0.6250000000000000  0.7473850000000013  0.3553115827490103   F   F   F
  0.6250000000000000  0.2526149999999987  0.2726324871770203   F   F   F
  0.8750000000000000  0.7473850000000013  0.4793302261070025   F   F   F
  0.8750000000000000  0.2526149999999987  0.3966511305350124   F   F   F
  0.6262323168894367  0.7334626452724875  0.6011410505974319   T   T   T
  0.6254875441092305  0.2511242664234892  0.5211775027531488   T   T   T
  0.8751680008558107  0.7271590473601250  0.7206623104703946   T   T   T
  0.8749327173244110  0.2231903198253529  0.6534664396199252   T   T   T
```

Figure 6. (110)-I

```
O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   O    La
    19    12
Selective dynamics
Direct
  0.4086274080959859  0.0326709792418299  0.7200049680498929   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.4963938256254155  0.5088730662462578  0.5349674580936968   T   T   T
  0.8334073266901347  0.8426885922215803  0.5406804081279527   T   T   T
  0.1591735590517034  0.1476708651528449  0.5391806786257437   T   T   T
 -0.0341142197276698  0.4346752483226327  0.6369847838996254   T   T   T
  0.2898712565614656  0.8352329820046444  0.6198275974862308   T   T   T
  0.6355029088662836  0.1236236285674512  0.6148675033303160   T   T   T
  0.4880923795288899  0.4855761709625802  0.6793048181508310   T   T   T
  0.8541063440228855  0.8713274086374287  0.6922718873048734   T   T   T
```

```
  0.2019809669871192  0.1158902544090154  0.7173730250553806   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8229369977812101  0.2406061915857259  0.5407591797637902   T   T   T
  0.1658677306779541  0.7436530304620274  0.5352390916557010   T   T   T
  0.3004723012651684  0.2314398385396159  0.6261367174682401   T   T   T
  0.6522038727459105  0.7338430319448639  0.6212104762078691   T   T   T
  0.7527137782416071  0.2272689339906522  0.6957723181167870   T   T   T
  0.1733777736835518  0.7380176534327967  0.6994212680182268   T   T   T
```

Figure 6. (110)-II

```
O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   O    La
    19    12
Selective dynamics
Direct
  0.4869126581372896  0.3335151819696508  0.7218155956207974   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.5064682526254849  0.5158766010547289  0.5354176176527241   T   T   T
  0.8407485830243472  0.8550634399282812  0.5389351169077076   T   T   T
  0.1691142702737600  0.1507857134848667  0.5406430927166590   T   T   T
 -0.0076944475132507  0.5008886303043504  0.6260598215348928   T   T   T
  0.3206312469091068  0.8474760292667378  0.6206510731537268   T   T   T
  0.6612242705038117  0.1402978824627842  0.6161280631170352   T   T   T
  0.4882557194453225  0.5168169718511495  0.6833463525265746   T   T   T
  0.8207668426967373  0.8507931483105529  0.6973313940724922   T   T   T
  0.1330206464537658  0.1163193756106390  0.6975662506070422   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8339149841591355  0.2505722697101256  0.5380369619583031   T   T   T
  0.1718881269527541  0.7469707897973112  0.5382270310713481   T   T   T
  0.3193981813373382  0.2414359227639438  0.6262655307919737   T   T   T
  0.6657052007600915  0.7436118629786426  0.6175323917367479   T   T   T
  0.8110564564541026  0.2289300327729001  0.6948540863989290   T   T   T
  0.1434910142776041  0.7529965243021063  0.6946622541958016   T   T   T
```

Figure 6. (110)-III

```
O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   O    La
    19    12
Selective dynamics
Direct
  0.0958597534804358  0.1233096744298352  0.7581592289399681   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.4875581986349503  0.5057090031047560  0.5412854513884932   T   T   T
  0.8389855896428066  0.8479660761707452  0.5381596322278028   T   T   T
  0.1707190065142516  0.1430162238519766  0.5390043106825396   T   T   T
 -0.0156932979684754  0.4602110929785110  0.6207184489900968   T   T   T
  0.3113632432007416  0.8616486250174504  0.6257763340567787   T   T   T
  0.6591240088759748  0.1309386221269432  0.6151464684917896   T   T   T
  0.5385406447666888  0.4791230357945092  0.6798011589363533   T   T   T
  0.8629710865736053  0.8660619985686424  0.6896031280631718   T   T   T
  0.1811391519805791  0.1821317329667101  0.7053632103205189   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8381215287108197  0.2484240864916723  0.5391032103660396   T   T   T
  0.1696765795178393  0.7530515950026732  0.5396768868800380   T   T   T
  0.3352802691210155  0.2691595121044268  0.6200795991235994   T   T   T
  0.6627007498323830  0.7441150728551961  0.6191591237816459   T   T   T
  0.8216176271989992  0.2566896716940147  0.6908517634498613   T   T   T
  0.1671827656321794  0.7954136022292692  0.7052437558984863   T   T   T
```

Figure 6. (110)-IV

```
O La
   1.00000000000000
     6.8233968359095165    0.0000000000000000    0.0000000000000000
     0.0000000000000000    6.1837999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   24.8487250000000017
   O    La
    19    12
Selective dynamics
Direct
  0.4999662998361117  0.4998366839023096  0.7389462725873350   T   T   T
  0.0000000000000000  0.5000000000000000  0.3018263512514210   F   F   F
  0.3333333333333357  0.8545579999999973  0.3018263512514210   F   F   F
  0.6666666666666643  0.1454420000000027  0.3018263512514210   F   F   F
```

```
  0.5000000000000000  0.5000000000000000  0.3810958107508498   F   F   F
  0.8333333333333357  0.8545579999999973  0.3810958107508498   F   F   F
  0.1666666666666643  0.1454420000000027  0.3810958107508498   F   F   F
  0.0000000000000000  0.5000000000000000  0.4603652702502856   F   F   F
  0.3333333333333357  0.8545579999999973  0.4603652702502856   F   F   F
  0.6666666666666643  0.1454420000000027  0.4603652702502856   F   F   F
  0.5000056027446061  0.5000042328827382  0.5362155457175830   T   T   T
  0.8375621520710925  0.8527203570235780  0.5391901942141590   T   T   T
  0.1624461199107463  0.1472937955127217  0.5391927798448948   T   T   T
  0.0000078083203199  0.5000078929695156  0.6271985858921564   T   T   T
  0.3287747431075737  0.8570665423056558  0.6196184142919454   T   T   T
  0.6712172799357481  0.1429340155006978  0.6196210211658735   T   T   T
  0.5000015589661094  0.5000598706529344  0.6791859291772320   T   T   T
  0.8451332103448217  0.8646587248293367  0.6984011122654821   T   T   T
  0.1548270766192287  0.1353073502591278  0.6983960332028223   T   T   T
  0.3333333333333357  0.2526149999999987  0.3018263512514210   F   F   F
  0.6666666666666643  0.7473850000000013  0.3018263512514210   F   F   F
  0.8333333333333357  0.2526149999999987  0.3810958107508498   F   F   F
  0.1666666666666643  0.7473850000000013  0.3810958107508498   F   F   F
  0.3333333333333357  0.2526149999999987  0.4603652702502856   F   F   F
  0.6666666666666643  0.7473850000000013  0.4603652702502856   F   F   F
  0.8287147210112967  0.2516465199209841  0.5385103673351120   T   T   T
  0.1712870597501242  0.7483520401425067  0.5385099814995523   T   T   T
  0.3205133537677726  0.2477719699930189  0.6212337135684308   T   T   T
  0.6794769538271077  0.7522220315392112  0.6212288175577234   T   T   T
  0.8250096478640885  0.2391598489742209  0.6974523644977751   T   T   T
  0.1749561182902434  0.7608164987941136  0.6974465017779771   T   T   T
```

Figure 6. (101)-I

```
O La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   O    La
    25    16
Selective dynamics
Direct
  0.2673930133172473  0.1889732782192791  0.7106141470086581   T   T   T
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.0967894657056954  0.4839910110861049  0.5588646104053022   T   T   T
  0.4378411641764930  0.1415933093427112  0.5512082578646137   T   T   T
  0.7465510475282455  0.3138684322815693  0.5628972335677664   T   T   T
  0.3163708650831000  0.1732531116429560  0.6554489572444687   T   T   T
  0.6246699655049616  0.3416129951475878  0.6722293706236985   T   T   T
  0.9044193020072936  0.0209118332573711  0.6752113743906013   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
```

```
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.0973378796793464  0.9680209602327183  0.5564872581044127   T   T   T
  0.4464785581991787  0.6379958818166348  0.5486786740912439   T   T   T
  0.7399566281880613  0.8152329042304374  0.5617721447301477   T   T   T
  0.3257645624542305  0.6673359026260383  0.6540333842912943   T   T   T
  0.6186632021290173  0.8487088047229802  0.6709079253531739   T   T   T
  0.8841571482116830  0.5331779859196089  0.6760412458619317   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7418765354899185  0.0651169796506724  0.5105483870739199   T   T   T
  0.4149931278840827  0.4023520762405837  0.5978664165869145   T   T   T
  0.9558614960155967  0.2639275265863585  0.6344689947258094   T   T   T
  0.6049252604414282  0.0976528046517828  0.7101543013227585   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7452800126795768  0.5638070812036046  0.5092894836799131   T   T   T
  0.4110920082778213  0.8918071560229970  0.5974901102029727   T   T   T
  0.9589790542429337  0.7588971944780531  0.6298076108686359   T   T   T
  0.5794771480542980  0.6069554991475891  0.7061610763144841   T   T   T
```

Figure 6. (101)-II

```
O La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   O    La
    25    16
Selective dynamics
Direct
  0.9125233386058604  0.1223977562280547  0.7268741109109584   T   T   T
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.0877954687941670  0.4964036630136237  0.5633762037689094   T   T   T
  0.4377612968205202  0.1421971483290373  0.5487928252001951   T   T   T
  0.7535896785825296  0.3108167575897433  0.5628886757812890   T   T   T
  0.3174678154666363  0.1738945243123900  0.6554667618102993   T   T   T
  0.6244138331032423  0.3412486332424409  0.6688466294480055   T   T   T
  0.9086933544170260  0.0090446814899363  0.6818973286864372   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.0944599419172203  0.9629897988962782  0.5591393816107157   T   T   T
  0.4443095143171161  0.6386710405098877  0.5489006474313164   T   T   T
  0.7382878402929993  0.8172943302633257  0.5624634546190292   T   T   T
```

```
  0.3286839583350268  0.6676064152401457  0.6552580960615298   T   T   T
  0.6227250711811179  0.8493664842849358  0.6719505511684963   T   T   T
  0.8937512671309312  0.5315975765335883  0.6752350851883460   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7424670931223172  0.0659699808443631  0.5106200194187475   T   T   T
  0.4152013357232898  0.3968340824995222  0.5985884673289620   T   T   T
  0.9670226119762471  0.2616208839249872  0.6370068686517908   T   T   T
  0.5826242381192455  0.1081411512672380  0.7087351775669808   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7413104902205245  0.5640291829363432  0.5106133200512886   T   T   T
  0.4101020462633431  0.8980789319973517  0.5992199391262485   T   T   T
  0.9674898897315477  0.7492831978297296  0.6265622254219007   T   T   T
  0.5909220180152194  0.6021903083128834  0.7054078354568535   T   T   T
```

Figure 6. (101)-III

```
O  La
   1.00000000000000
     7.3320504567344598    0.0000000000000000    0.0000000000000000
     2.1166768493587393    7.5893349481880668    0.0000000000000000
     0.0000000000000000    0.0000000000000000   26.4666250656236741
   O    La
    25    16
Selective dynamics
Direct
  0.6784160650619623  0.3310943952024920  0.7403706025567740   T   T   T
  0.6166790643543223  0.0958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.2584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.4332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.2874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.4500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.1248919646103062  0.4459618958584386   F   F   F
  0.1044668538936006  0.4751566928227297  0.5602048058343996   T   T   T
  0.4417120139350189  0.1435493515914831  0.5495968072644128   T   T   T
  0.7438385873931282  0.3148644407669280  0.5677786507158862   T   T   T
  0.3269379487288395  0.1700823316315101  0.6570452040027343   T   T   T
  0.6380119753954836  0.3407343315233501  0.6840149619736003   T   T   T
  0.8930564603667344  0.0230943156923009  0.6750059421388985   T   T   T
  0.6166790643543223  0.5958302339114212  0.3306989717953783   F   F   F
  0.9662841158585209  0.7584289710353715  0.3283033998687301   F   F   F
  0.2670740128501166  0.9332314967874709  0.3330945437220194   F   F   F
  0.8500371930629598  0.7874907017342565  0.4435663239317904   F   F   F
  0.1996422445671584  0.9500894388582140  0.4411707520051493   F   F   F
  0.5004321415587540  0.6248919646103133  0.4459618958584386   F   F   F
  0.0958781070611767  0.9736188029287070  0.5569036854631672   T   T   T
  0.4425737917677183  0.6349624968251439  0.5492285106152458   T   T   T
  0.7429953147077596  0.8130749384727612  0.5591713643612575   T   T   T
  0.3318730791416010  0.6658158607086493  0.6562049860796946   T   T   T
  0.6303310626808929  0.8438142286975933  0.6640224385606662   T   T   T
  0.8907801548132780  0.5319625398440680  0.6745443590079101   T   T   T
  0.2714512792191499  0.1821371801952125  0.2833757602793625   F   F   F
```

```
  0.9619068494894876  0.0095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.3737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.2011837554504723  0.4908895354477991   F   F   F
  0.7421585401189010  0.0666605119235860  0.5103847009535295   T   T   T
  0.4095394479168951  0.3983915047365169  0.6000241447879231   T   T   T
  0.9698071214249422  0.2588163929248911  0.6351005836666851   T   T   T
  0.5847119264352546  0.0844500193290257  0.7089120349623299   T   T   T
  0.2714512792191499  0.6821371801952125  0.2833757602793625   F   F   F
  0.9619068494894876  0.5095232876276299  0.3780221833113870   F   F   F
  0.5048094079277874  0.8737976480180549  0.3962431124157817   F   F   F
  0.1952649781981322  0.7011837554504723  0.4908895354477991   F   F   F
  0.7405800047523464  0.5622228784232646  0.5099227830528734   T   T   T
  0.4108298902132257  0.8963918596055592  0.5962833853419038   T   T   T
  0.9577615064291176  0.7607123077994773  0.6289699717901819   T   T   T
  0.5825087045954578  0.6248579146818596  0.7086542337250927   T   T   T
```

Figure 6. (111)-I

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O
    12    19
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5431503487639271  0.5263888725204960  0.2661457388916249   T   T   T
  0.0461466288655999  0.5623878927803148  0.3558414976711930   T   T   T
  0.6343787976193754  0.7834507813771718  0.3988497980842702   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1091930311288729  0.9727194043952589  0.2232683746832994   T   T   T
  0.6446540073055537  0.0660264530846362  0.2944918342216074   T   T   T
  0.1937497704977862  0.1187934446188914  0.3702689086836861   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3655583378068819  0.7590032934704128  0.2376322577310569   T   T   T
  0.8231598523375937  0.8220173279369773  0.3180656501066378   T   T   T
  0.3801333322063450  0.8866279657510099  0.3662619707074661   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8405162742692739  0.0858452320434166  0.2167817484784086   T   T   T
  0.3549623093866632  0.1673010881294724  0.2904564644472010   T   T   T
  0.8915599371313202  0.1876283585497616  0.3710845777742562   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
  0.8456554786792354  0.4357658515717845  0.2759849103848624   T   T   T
  0.3644804944445391  0.4865847929782016  0.3592207737169346   T   T   T
  0.9875370332776032  0.8074068714208431  0.4250838799360781   T   T   T
```

```
  0.8178842604548074  0.5861498055648086  0.4262715692377580   T   T   T
```

Figure 6. (111)-II

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O
    12    19
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5564091864499339  0.5297505493961513  0.2630329810789271   T   T   T
  0.0310319346453073  0.5457613401487446  0.3631476998775773   T   T   T
  0.6307263952191534  0.7991837459860875  0.4034505368245248   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1083457185308247  0.9769556496561596  0.2240935142637632   T   T   T
  0.6402076679196529  0.0589768303645736  0.2935597521463988   T   T   T
  0.1743133354552441  0.0894177792514306  0.3703081277680285   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3759656310927035  0.7590005447371933  0.2366471581947852   T   T   T
  0.8223198206090967  0.8380838299402765  0.3112041967820934   T   T   T
  0.3588160203388229  0.8712638035318812  0.3655282444652461   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8419042880938136  0.0916485727822073  0.2156940751595769   T   T   T
  0.3548355653878459  0.1684873965620212  0.2907478920096842   T   T   T
  0.8605654049607754  0.1663463086619405  0.3764497957137037   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
  0.8502552199801573  0.4349374032554712  0.2786746969759836   T   T   T
  0.3746560951561405  0.4806255351082029  0.3582009924829017   T   T   T
  0.9335612320517834  0.7595082937462486  0.4139196846859820   T   T   T
  0.3065684146589928  0.4547160557792801  0.4143434482108956   T   T   T
```

Figure 6. (111)-III

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O
    12    19
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
```

```
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5517033494016117  0.5214818986100270  0.2663956701018371   T   T   T
  0.1046687288530019  0.5864124421237443  0.3495413258789827   T   T   T
  0.6868238121898375  0.7996128382575035  0.3983784185821501   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1060859051355421  0.9746796278591815  0.2251102121142126   T   T   T
  0.6460082626837932  0.0604228572828829  0.2919884371256339   T   T   T
  0.2495576280872965  0.1278501779775197  0.3794688784189245   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3594525258285790  0.7592611601314780  0.2430222435671620   T   T   T
  0.8089652865445277  0.8312561494866423  0.3079793192010873   T   T   T
  0.4271914338094265  0.9093542819094189  0.3688859591149634   T   T   T
  0.1953125813377383  0.8018515466180745  0.0000000000000000   F   F   F
  0.7413508490531768  0.8938395122850622  0.0729924168773124   F   F   F
  0.2873782264472950  0.9859815616466321  0.1459848337546177   F   F   F
  0.8401154754216287  0.0884661006621535  0.2141065331184739   T   T   T
  0.3527561700719036  0.1617253074651504  0.2929753307331273   T   T   T
  0.9207242850398891  0.1959076539299544  0.3710171192922685   T   T   T
  0.2067639675224910  0.1579357869491815  0.0517596733424099   F   F   F
  0.7527327231151588  0.2500778363107514  0.1247520902197152   F   F   F
  0.2989066550128996  0.3422198856723213  0.1977445070970276   F   F   F
  0.8543553249297849  0.4338470148128635  0.2762401466149648   T   T   T
  0.4048960829585156  0.4932398504991861  0.3636595706298461   T   T   T
  0.9917244997032187  0.7579479062164249  0.4043594143475883   T   T   T
  0.9549727599935985  0.1637342991063245  0.4270743082780246   T   T   T
```

Figure 6. (111)-IV

```
O La
   1.00000000000000
     6.8234000000000004    0.0000000000000000    0.0000000000000000
    -3.4117236276940459    6.4899793757942073    0.0000000000000000
     0.0000000000000016    0.0000000000000026   25.7149999999999999
   La   O
    12    19
Selective dynamics
Direct
  0.9219846346797027  0.2553166819266224  0.0439432237993387   F   F   F
  0.4681585665774435  0.3474587312881923  0.1169356406766511   F   F   F
  0.0141859439715617  0.4396007806497622  0.1898891697452854   F   F   F
  0.5445353849956289  0.5221981034594627  0.2664781620245307   T   T   T
  0.0389343555283244  0.5365401217408904  0.3589829452368120   T   T   T
  0.6500211871334574  0.7840178094015786  0.4011631167530947   T   T   T
  0.4800332923790691  0.7044706516406336  0.0078164495430713   F   F   F
  0.0260606697731873  0.7966127010022035  0.0808088664203765   F   F   F
  0.5721759798694777  0.8887547503637734  0.1538012832976889   F   F   F
  0.1081040647689038  0.9716051210288252  0.2243990808348483   T   T   T
  0.6526368389641198  0.0611236425868437  0.2922508759714652   T   T   T
  0.2047050744760343  0.1134576104154418  0.3737377274819717   T   T   T
  0.7009704423389636  0.4798166249363334  0.0258603927668659   F   F   F
  0.2469978197330818  0.5719586742979033  0.0988528096441783   F   F   F
  0.7931131298293721  0.6641007236594731  0.1718452265214836   F   F   F
  0.3698779284224296  0.7630217486711494  0.2390240728108125   T   T   T
```

0.8089204120719016	0.8285037990293532	0.3100545212507611	T	T	T
0.3756703666766332	0.8825895279656023	0.3654667625966742	T	T	T
0.1953125813377383	0.8018515466180745	0.0000000000000000	F	F	F
0.7413508490531768	0.8938395122850622	0.0729924168773124	F	F	F
0.2873782264472950	0.9859815616466321	0.1459848337546177	F	F	F
0.8431234470672618	0.0902010648614056	0.2150614881576724	T	T	T
0.3547266482755227	0.1617307663328567	0.2919169945240237	T	T	T
0.8954360006361497	0.1766635835169396	0.3742356423715060	T	T	T
0.2067639675224910	0.1579357869491815	0.0517596733424099	F	F	F
0.7527327231151588	0.2500778363107514	0.1247520902197152	F	F	F
0.2989066550128996	0.3422198856723213	0.1977445070970276	F	F	F
0.8493813555859998	0.4311192207567600	0.2774968756599135	T	T	T
0.3739862399101446	0.4823638923477132	0.3640891806169650	T	T	T
0.9356967477133450	0.7285849255434850	0.4113405360278266	T	T	T
0.4209802964911046	0.9615015785403693	0.4200963562523307	T	T	T