

Supporting Information for Structure and stability of the (001) α -quartz surface

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PW91 Surface energies (J/m²)

Surface	Depth	PW91
cleaved	18 layers	2.20
reconstructed	27 layers	0.37
hydroxylated	18 layers	0.19

Structures

L=Large basis set, see computational details in text.

Where only surface vectors are provided (B3LYP surfaces), z-coordinates are absolute.

Bulk B3LYP/6-31G*

cell vectors

4.33313034	-2.50173397	0.00000000
-0.00000000	5.00346794	0.00000000
0.00000000	0.00000000	5.50385541

fractional coordinates

Si	0.47109730	-0.00000000	0.33333333
Si	0.00000000	0.47109730	-0.33333333
Si	-0.47109730	-0.47109730	0.00000000
O	0.41465454	0.26644586	0.21336923
O	-0.26644586	0.14820868	-0.45329744
O	-0.14820868	-0.41465454	-0.11996410
O	0.14820868	-0.26644586	0.45329744
O	-0.41465454	-0.14820868	0.11996410
O	0.26644586	0.41465454	-0.21336923

Bulk B3LYP/L

cell vectors

4.33909802	-2.50517941	0.00000000
0.00000000	5.01035882	0.00000000
0.00000000	0.00000000	5.49755440

fractional coordinates

Si	0.47187287	0.00000000	0.33333333
Si	-0.00000000	0.47187287	-0.33333333
Si	-0.47187287	-0.47187287	0.00000000
O	0.41477567	0.26455347	0.21188160
O	-0.26455347	0.15022220	-0.45478506
O	-0.15022220	-0.41477567	-0.12145173
O	0.15022220	-0.26455347	0.45478506
O	-0.41477567	-0.15022220	0.12145173
O	0.26455347	0.41477567	-0.21188160

Bulk PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	5.54678160

fractional coordinates

O	0.41529600	0.25166200	0.29820500
O	0.74833800	0.16363500	0.96487200
O	0.83636500	0.58470400	0.63153800
O	0.16363500	0.74833800	0.03512800
O	0.58470400	0.83636500	0.36846100
O	0.25166200	0.41529600	0.70179500
Si	0.47865900	0.00000000	0.16666700
Si	0.00000000	0.47865900	0.83333300
Si	0.52134100	0.52134100	0.50000000

Bulk PW91

cell vectors

5.05617610	0.00000000	0.00000000
-2.52808800	4.37877690	0.00000000
0.00000000	0.00000000	5.56103770

fractional coordinates

O	0.41600800	0.24951100	0.30036900
O	0.75048900	0.16649700	0.96703600
O	0.83350300	0.58399200	0.63370200
O	0.16649700	0.75048900	0.03296400
O	0.58399200	0.83350300	0.36629700
O	0.24951100	0.41600800	0.69963100
Si	0.47962400	0.00000000	0.16666700
Si	0.00000000	0.47962400	0.83333300
Si	0.52037600	0.52037600	0.50000000

Cleaved surface 18 layers B3LYP/6-31G*

surface vectors

5.00346790	0.00000000
-2.50173400	4.33313030

fractional coordinates

O	0.24578910	0.41833927	-0.27027901
O	-0.17255018	-0.41833927	0.27027901
Si	-0.02594862	0.46784864	-0.91458516
Si	-0.49379727	-0.46784864	0.91458516
O	-0.29354803	0.14320102	-1.55260211
O	-0.43674906	-0.14320102	1.55260211
O	0.11739320	-0.26613074	-2.08959272
O	0.38352394	0.26613074	2.08959272
Si	0.44747418	-0.00844910	-2.75265355
Si	0.45592328	0.00844910	2.75265355
O	0.40697773	0.26896861	-3.41577451
O	0.13800912	-0.26896861	3.41577451
O	-0.42735399	-0.15781531	-3.85708514
O	-0.26953868	0.15781531	3.85708514
Si	-0.35575612	-0.42622569	-4.29350070

Si	0.07046958	0.42622569	4.29350070
O	-0.09146333	-0.39260845	-5.16832816
O	0.30114513	0.39260845	5.16832816

Cleaved surface 18 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

O	0.24290897	0.41724113	-0.25544545
O	-0.17433216	-0.41724113	0.25544545
Si	-0.02505823	0.46958247	-0.91686595
Si	-0.49464070	-0.46958247	0.91686595
O	-0.29006394	0.14621045	-1.57027703
O	-0.43627439	-0.14621045	1.57027703
O	0.12260154	-0.26368956	-2.08227167
O	0.38629110	0.26368956	2.08227167
Si	0.44975713	-0.00766247	-2.76150609
Si	0.45741960	0.00766247	2.76150609
O	0.40757067	0.26726436	-3.43574299
O	0.14030630	-0.26726436	3.43574299
O	-0.42831226	-0.15930928	-3.86708071
O	-0.26900298	0.15930928	3.86708071
Si	-0.35977286	-0.42798187	-4.31386010
Si	0.06820901	0.42798187	4.31386010
O	-0.09623262	-0.39485841	-5.19393634
O	0.29862579	0.39485841	5.19393634

Cleaved surface 27 layers B3LYP/6-31G*
surface vectors

5.00346790 0.00000000
-2.50173400 4.33313030

fractional coordinates

Si	0.45580539	-0.00000000	0.00000000
O	0.39524283	0.25896334	-0.70401514
O	0.13627949	-0.25896334	0.70401514
O	-0.43212404	-0.15514008	-1.14858227
O	-0.27698395	0.15514008	1.14858227
Si	-0.48920545	-0.47325899	-1.85189212
Si	-0.01594645	0.47325899	1.85189212
O	-0.16707429	-0.41367179	-2.52808930
O	0.24659751	0.41367179	2.52808930
O	0.24921088	0.41876024	-3.02656570
O	-0.16954937	-0.41876024	3.02656570
Si	-0.01960492	0.46919788	-3.69333073
Si	-0.48880281	-0.46919788	3.69333073
O	-0.28694899	0.14405396	-4.32873008
O	-0.43100295	-0.14405396	4.32873008
O	0.12639651	-0.26718124	-4.87681006
O	0.39357775	0.26718124	4.87681006

Si	0.45636346	-0.00884531	-5.53627977
Si	0.46520877	0.00884531	5.53627977
O	0.41516970	0.26749826	-6.20730739
O	0.14767144	-0.26749826	6.20730739
O	-0.41595405	-0.15752466	-6.63228710
O	-0.25842938	0.15752466	6.63228710
Si	-0.34608572	-0.42670942	-7.07662066
Si	0.08062371	0.42670942	7.07662066
O	-0.08194831	-0.39346514	-7.95147694
O	0.31151684	0.39346514	7.95147694

Cleaved surface 27 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

Si	0.45648832	-0.00000000	0.00000000
O	0.39643121	0.25990127	-0.69536811
O	0.13652994	-0.25990127	0.69536811
O	-0.43195333	-0.15457860	-1.15158177
O	-0.27737473	0.15457860	1.15158177
Si	-0.48854065	-0.47325723	-1.84550141
Si	-0.01528342	0.47325723	1.84550141
O	-0.16639920	-0.41429878	-2.51585094
O	0.24789958	0.41429878	2.51585094
O	0.25027623	0.41832708	-3.02009810
O	-0.16805085	-0.41832708	3.02009810
Si	-0.01716854	0.47134892	-3.68272415
Si	-0.48851746	-0.47134892	3.68272415
O	-0.28237008	0.14781046	-4.33431997
O	-0.43018053	-0.14781046	4.33431997
O	0.13113694	-0.26224947	-4.84939865
O	0.39338641	0.26224947	4.84939865
Si	0.45829989	-0.00651327	-5.52866953
Si	0.46481316	0.00651327	5.52866953
O	0.41622172	0.26801458	-6.20792100
O	0.14820714	-0.26801458	6.20792100
O	-0.41885675	-0.15816055	-6.63014183
O	-0.26069620	0.15816055	6.63014183
Si	-0.35048302	-0.42668893	-7.08135854
Si	0.07620591	0.42668893	7.08135854
O	-0.08666584	-0.39330993	-7.96039954
O	0.30664409	0.39330993	7.96039954

Cleaved surface 36 layers B3LYP/6-31G*
surface vectors

5.00346790 0.00000000
-2.50173400 4.33313030

fractional coordinates

O	0.24641640	0.41382909	-0.23556060
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O	-0.16741270	-0.41382909	0.23556060
Si	-0.01582074	0.47210887	-0.92230350
Si	-0.48792962	-0.47210887	0.92230350
O	-0.27909298	0.15130728	-1.60284230
O	-0.43040026	-0.15130728	1.60284230
O	0.13657624	-0.26433372	-2.08817256
O	0.40090997	0.26433372	2.08817256
Si	0.45775710	-0.00213822	-2.76981155
Si	0.45989532	0.00213822	2.76981155
O	0.39909564	0.25889193	-3.46658982
O	0.14020371	-0.25889193	3.46658982
O	-0.42695110	-0.15437647	-3.91898328
O	-0.27257463	0.15437647	3.91898328
Si	-0.48424042	-0.47341997	-4.61579620
Si	-0.01082044	0.47341997	4.61579620
O	-0.16191663	-0.41468314	-5.28711891
O	0.25276652	0.41468314	5.28711891
O	0.25453930	0.41779150	-5.79271262
O	-0.16325221	-0.41779150	5.79271262
Si	-0.01579857	0.46677396	-6.45311539
Si	-0.48257254	-0.46677396	6.45311539
O	-0.28420125	0.14079053	-7.07951958
O	-0.42499177	-0.14079053	7.07951958
O	0.12899637	-0.27035834	-7.64077430
O	0.39935472	0.27035834	7.64077430
Si	0.46012352	-0.01169600	-8.29233935
Si	0.47181952	0.01169600	8.29233935
O	0.42005987	0.26516682	-8.96404178
O	0.15489304	-0.26516682	8.96404178
O	-0.41130370	-0.16014231	-9.38494859
O	-0.25116139	0.16014231	9.38494859
Si	-0.34119350	-0.42892382	-9.83262153
Si	0.08773033	0.42892382	9.83262153
O	-0.07731242	-0.39512167	-10.71095885
O	0.31780926	0.39512167	10.71095885

Cleaved surface 36 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

O	0.25001015	0.41560141	-0.24140388
O	-0.16559127	-0.41560141	0.24140388
Si	-0.01171966	0.47498702	-0.92319585
Si	-0.48670668	-0.47498702	0.92319585
O	-0.27290946	0.15566112	-1.61785023
O	-0.42857058	-0.15566112	1.61785023
O	0.14129147	-0.25861092	-2.07443376
O	0.39990238	0.25861092	2.07443376
Si	0.46118154	0.00114696	-2.77104282

Si	0.46003459	-0.00114696	2.77104282
O	0.40087880	0.26065820	-3.47009371
O	0.14022060	-0.26065820	3.47009371
O	-0.42727648	-0.15366778	-3.92157940
O	-0.27360869	0.15366778	3.92157940
Si	-0.48551889	-0.47254520	-4.62044675
Si	-0.01297369	0.47254520	4.62044675
O	-0.16414274	-0.41285992	-5.30135215
O	0.24871718	0.41285992	5.30135215
O	0.25228857	0.41872821	-5.79082694
O	-0.16643964	-0.41872821	5.79082694
Si	-0.01548503	0.47025766	-6.46008526
Si	-0.48574269	-0.47025766	6.46008526
O	-0.28177971	0.14570625	-7.10104550
O	-0.42748596	-0.14570625	7.10104550
O	0.13269895	-0.26570079	-7.63835114
O	0.39839974	0.26570079	7.63835114
Si	0.46146790	-0.00936071	-8.30648261
Si	0.47082862	0.00936071	8.30648261
O	0.42125515	0.26545009	-8.99350862
O	0.15580506	-0.26545009	8.99350862
O	-0.41286613	-0.16047855	-9.39720861
O	-0.25238758	0.16047855	9.39720861
Si	-0.34325931	-0.42787655	-9.85439385
Si	0.08461724	0.42787655	9.85439385
O	-0.07920613	-0.39327844	-10.73518211
O	0.31407231	0.39327844	10.73518211

Reconstructed surface 18 layers B3LYP/6-31G*
surface vectors

5.00346790 0.00000000
-2.50173400 4.33313030

fractional coordinates

O	0.32536687	0.49983285	-0.39015820
O	-0.17446599	-0.49983285	0.39015820
Si	0.01752638	-0.49999920	-0.91935559
Si	-0.48247443	0.49999920	0.91935559
O	-0.18558415	0.19857461	-1.87829748
O	-0.38415876	-0.19857461	1.87829748
O	0.11634856	-0.19847476	-1.87858592
O	0.31482333	0.19847476	1.87858592
Si	-0.21172009	0.17220982	-3.52059701
Si	-0.38392991	-0.17220982	3.52059701
O	0.04863255	-0.49990235	-4.16484852
O	-0.45146511	0.49990235	4.16484852
O	-0.15457773	-0.10441508	-4.01149015
O	-0.05016265	0.10441508	4.01149015
Si	0.11635888	-0.17189247	-3.52082672
Si	0.28825135	0.17189247	3.52082672
O	0.44997870	0.10487112	-4.01266831

O 0.34510758 -0.10487112 4.01266831

Reconstructed surface 18 layers B3LYP/L

surface vectors

5.01035882 0.00000000

-2.50517941 4.33909802

fractional coordinates

O	0.32040900	0.49993454	-0.37115507
O	-0.17952554	-0.49993454	0.37115507
Si	0.01491635	0.49989916	-0.92587445
Si	-0.48498281	-0.49989916	0.92587445
O	-0.18353348	0.19991038	-1.89418227
O	-0.38344386	-0.19991038	1.89418227
O	0.11624510	-0.20006070	-1.89342160
O	0.31630580	0.20006070	1.89342160
Si	-0.21026600	0.17235387	-3.53658073
Si	-0.38261987	-0.17235387	3.53658073
O	0.04592732	0.49999161	-4.18555831
O	-0.45406429	-0.49999161	4.18555831
O	-0.15004311	-0.10124226	-4.02549318
O	-0.04880085	0.10124226	4.02549318
Si	0.11729828	-0.17244973	-3.53559303
Si	0.28974802	0.17244973	3.53559303
O	0.45108734	0.10126198	-4.02411830
O	0.34982536	-0.10126198	4.02411830

Reconstructed surface 27 layers B3LYP/6-31G*

surface vectors

5.00346790 0.00000000

-2.50173400 4.33313030

fractional coordinates

Si	0.46902749	-0.00000000	0.00000000
O	0.14804516	-0.24492982	0.74486145
O	0.39297499	0.24492982	-0.74486145
O	-0.25428158	0.16335476	1.10369146
O	-0.41763634	-0.16335476	-1.10369146
Si	0.00379978	0.47676032	1.84604435
Si	-0.47296054	-0.47676032	-1.84604435
O	0.28971792	0.44531059	2.44754700
O	-0.15559268	-0.44531059	-2.44754700
O	-0.15905978	-0.45168089	3.10047205
O	0.29262112	0.45168089	-3.10047205
Si	-0.48356553	0.49647414	3.70707597
Si	0.01996033	-0.49647414	-3.70707597
O	-0.40001897	-0.20547198	4.67170711
O	-0.19454699	0.20547198	-4.67170711
O	0.34154256	0.19523727	4.68969448
O	0.14630529	-0.19523727	-4.68969448
Si	-0.36160825	-0.18272239	6.31590956
Si	-0.17888586	0.18272239	-6.31590956

O	0.38262250	0.48842734	6.97202551
O	-0.10580484	-0.48842734	-6.97202551
O	-0.01988553	-0.11695866	6.74720769
O	0.09707313	0.11695866	-6.74720769
Si	0.31862975	0.16222159	6.32598623
Si	0.15640816	-0.16222159	-6.32598623
O	-0.41570613	0.09126970	6.86672391
O	0.49302417	-0.09126970	-6.86672391

Reconstructed surface 27 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

Si	0.46941440	-0.00000000	0.00000000
O	0.14792244	-0.24945019	0.72629585
O	0.39737263	0.24945019	-0.72629585
O	-0.25670652	0.15987607	1.11709909
O	-0.41658259	-0.15987607	-1.11709909
Si	0.00000189	0.47629780	1.84491726
Si	-0.47629592	-0.47629780	-1.84491726
O	0.28072050	0.44135177	2.47810929
O	-0.16063128	-0.44135177	-2.47810929
O	-0.16336061	-0.44602594	3.07453579
O	0.28266533	0.44602594	-3.07453579
Si	-0.48678782	0.49590413	3.71491390
Si	0.01730805	-0.49590413	-3.71491390
O	-0.40232612	-0.20869758	4.69237294
O	-0.19362854	0.20869758	-4.69237294
O	0.34782741	0.19566929	4.70421325
O	0.15215812	-0.19566929	-4.70421325
Si	-0.36186997	-0.18522191	6.33457363
Si	-0.17664806	0.18522191	-6.33457363
O	0.38666635	0.48592386	6.99293210
O	-0.09925751	-0.48592386	-6.99293210
O	-0.01936451	-0.11567017	6.75122774
O	0.09630566	0.11567017	-6.75122774
Si	0.31985797	0.16052190	6.34017880
Si	0.15933607	-0.16052190	-6.34017880
O	-0.41969785	0.08478723	6.89119576
O	0.49551492	-0.08478723	-6.89119576

Reconstructed surface 36 layers B3LYP/6-31G*
surface vectors

5.00346790 0.00000000
-2.50173400 4.33313030

fractional coordinates

O	-0.16879558	-0.40549943	0.20805060
O	0.23670385	0.40549943	-0.20805060
Si	-0.48912608	-0.46831649	0.91599530

Si	-0.02080958	0.46831649	-0.91599530
O	-0.43984560	-0.14861994	1.56929404
O	-0.29122566	0.14861994	-1.56929404
O	0.41442218	0.27906573	2.11839324
O	0.13535644	-0.27906573	-2.11839324
Si	0.47414975	0.01532845	2.77548835
Si	0.45882131	-0.01532845	-2.77548835
O	0.15808299	-0.22992593	3.55453049
O	0.38800893	0.22992593	-3.55453049
O	-0.23596290	0.16751087	3.82397186
O	-0.40347378	-0.16751087	-3.82397186
Si	0.01369066	0.48026106	4.60387122
Si	-0.46657041	-0.48026106	-4.60387122
O	0.29922049	0.44721666	5.19788704
O	-0.14799618	-0.44721666	-5.19788704
O	-0.15574203	-0.46125809	5.87083515
O	0.30551607	0.46125809	-5.87083515
Si	-0.47921282	0.49145263	6.46751147
Si	0.02933456	-0.49145263	-6.46751147
O	-0.39626730	-0.21114280	7.43354151
O	-0.18512449	0.21114280	-7.43354151
O	0.34232872	0.18930652	7.44476334
O	0.15302220	-0.18930652	-7.44476334
Si	-0.35927704	-0.18875761	9.07694741
Si	-0.17051942	0.18875761	-9.07694741
O	0.38472207	0.48227158	9.73065355
O	-0.09754951	-0.48227158	-9.73065355
O	-0.01764189	-0.12303844	9.50869752
O	0.10539655	0.12303844	-9.50869752
Si	0.32039306	0.15610187	9.08221517
Si	0.16429118	-0.15610187	-9.08221517
O	-0.41385805	0.08526992	9.62286100
O	-0.49912796	-0.08526992	-9.62286100

Reconstructed surface 36 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

O	-0.16659519	-0.40854609	0.20946026
O	0.24195091	0.40854609	-0.20946026
Si	-0.48570038	-0.46938879	0.91844055
Si	-0.01631159	0.46938879	-0.91844055
O	-0.43196817	-0.14904616	1.58210012
O	-0.28292200	0.14904616	-1.58210012
O	0.41503693	0.27513202	2.10894268
O	0.13990492	-0.27513202	-2.10894268
Si	0.47487156	0.01237110	2.77341127
Si	0.46250046	-0.01237110	-2.77341127
O	0.15644827	-0.23576296	3.52505502

O	0.39221123	0.23576296	-3.52505502
O	-0.24113188	0.16552052	3.84843967
O	-0.40665240	-0.16552052	-3.84843967
Si	0.00927823	0.48121095	4.60524908
Si	-0.47193272	-0.48121095	-4.60524908
O	0.29160312	0.44730088	5.22719108
O	-0.15569776	-0.44730088	-5.22719108
O	-0.15841288	-0.45129216	5.84934605
O	0.29287928	0.45129216	-5.84934605
Si	-0.48073591	0.49670784	6.47631336
Si	0.02255625	-0.49670784	-6.47631336
O	-0.39563409	-0.20749706	7.45205835
O	-0.18813703	0.20749706	-7.45205835
O	0.34899339	0.19628674	7.46355798
O	0.15270665	-0.19628674	-7.46355798
Si	-0.35791353	-0.18438688	9.09578486
Si	-0.17352665	0.18438688	-9.09578486
O	0.38987681	0.48686454	9.75267744
O	-0.09698773	-0.48686454	-9.75267744
O	-0.01579754	-0.11504398	9.51944699
O	0.09924644	0.11504398	-9.51944699
Si	0.32272875	0.16124330	9.10007860
Si	0.16148545	-0.16124330	-9.10007860
O	-0.41596234	0.08601546	9.64486366
O	0.49802219	-0.08601546	-9.64486366

Hydrogenated surface 18 layers B3LYP/6-31G*
surface vectors

5.00346794 0.00000000
-2.50173397 4.33313034

fractional coordinates

H	-0.37713079	-0.43830743	-5.62485709
H	0.06117664	0.43830743	5.62485709
H	0.10083017	0.14232876	-5.57818609
H	-0.04149859	-0.14232876	5.57818609
O	-0.16534400	-0.36399260	5.38547596
O	0.19864859	0.36399260	-5.38547596
O	-0.45807856	-0.13166524	4.06104925
O	-0.32641332	0.13166524	-4.06104925
O	0.45306691	0.31926615	3.33180306
O	0.13380076	-0.31926615	-3.33180306
O	0.18126900	-0.21576282	1.95991187
O	0.39703182	0.21576282	-1.95991187
O	-0.21422153	0.17598624	1.73836076
O	-0.39020777	-0.17598624	-1.73836076
O	0.29536311	0.43426034	0.28433500
O	-0.13889722	-0.43426034	-0.28433500
O	-0.15297602	-0.35988701	-5.61873800
O	0.20691100	0.35988701	5.61873800
Si	-0.49467768	-0.45638951	4.61545593

Si	-0.03828817	0.45638951	-4.61545593
Si	0.49021395	0.03498769	2.75782464
Si	0.45522626	-0.03498769	-2.75782464
Si	0.02898452	0.48967211	0.93714285
Si	-0.46068759	-0.48967211	-0.93714285

Hydrogenated surface 18 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

H	-0.36950125	-0.43117884	-5.66133315
H	0.06167759	0.43117884	5.66133315
H	0.11517425	0.16027875	-5.64935087
H	-0.04510451	-0.16027875	5.64935087
O	-0.16985793	-0.37947663	5.41296923
O	0.20961870	0.37947663	-5.41296923
O	-0.45341268	-0.14267621	4.04190296
O	-0.31073647	0.14267621	-4.04190296
O	0.44612586	0.30321691	3.37274783
O	0.14290894	-0.30321691	-3.37274783
O	0.17138049	-0.22867562	1.99538107
O	0.40005611	0.22867562	-1.99538107
O	-0.22838505	0.16742349	1.70528621
O	-0.39580854	-0.16742349	-1.70528621
O	0.28106943	0.42858673	0.26165695
O	-0.14751730	-0.42858673	-0.26165695
O	-0.14657856	-0.35955435	-5.67078140
O	0.21297579	0.35955435	5.67078140
Si	-0.49558698	-0.46601066	4.63474267
Si	-0.02957632	0.46601066	-4.63474267
Si	0.48424888	0.02264892	2.76590567
Si	0.46159996	-0.02264892	-2.76590567
Si	0.01714774	0.48461246	0.93523301
Si	-0.46746472	-0.48461246	-0.93523301

Hydrogenated surface 27 layers B3LYP/6-31G*
surface vectors

5.00346794 0.00000000
-2.50173397 4.33313034

fractional coordinates

Si	0.48314117	0.00000000	0.00000000
O	0.42134610	0.25973602	-0.69047447
O	0.16161008	-0.25973602	0.69047447
O	-0.40325220	-0.15316876	-1.15254377
O	-0.25008344	0.15316876	1.15254377
Si	-0.46055636	-0.47298216	-1.84210369
Si	0.01242581	0.47298216	1.84210369
O	-0.14170102	-0.42303730	-2.50701414
O	0.28133628	0.42303730	2.50701414

O	0.28244659	0.42366718	-3.03043938
O	-0.14122059	-0.42366718	3.03043938
Si	0.02324364	0.48852408	-3.70144636
Si	-0.46528043	-0.48852408	3.70144636
O	-0.22142364	0.17392936	-4.49124234
O	-0.39535300	-0.17392936	4.49124234
O	0.17820852	-0.22120647	-4.74480330
O	0.39941499	0.22120647	4.74480330
Si	0.48681736	0.03328793	-5.52968268
Si	0.45352942	-0.03328793	5.52968268
O	0.44944972	0.31755181	-6.10301273
O	0.13189791	-0.31755181	6.10301273
O	-0.45742280	-0.13103161	-6.83143234
O	-0.32639119	0.13103161	6.83143234
Si	-0.49643660	-0.45692579	-7.38516823
Si	-0.03951082	0.45692579	7.38516823
O	-0.16705745	-0.36553979	-8.15298896
O	0.19848234	0.36553979	8.15298896
O	-0.15462200	-0.36039073	8.39169314
O	0.20576872	0.36039073	-8.39169314
H	-0.37860418	-0.43783651	8.39447995
H	0.05923233	0.43783651	-8.39447995
H	0.10077186	0.14407319	8.34900602
H	-0.04330132	-0.14407319	-8.34900602

Hydrogenated surface 27 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

Si	0.48014418	0.00000000	0.00000000
O	0.41897818	0.26032784	-0.68463504
O	0.15865034	-0.26032784	0.68463504
O	-0.40745100	-0.15331314	-1.15511377
O	-0.25413786	0.15331314	1.15511377
Si	-0.46631974	-0.47400114	-1.83976640
Si	0.00768141	0.47400114	1.83976640
O	-0.14755800	-0.42190352	-2.51345488
O	0.27434551	0.42190352	2.51345488
O	0.27361541	0.41941253	-3.01448316
O	-0.14579713	-0.41941253	3.01448316
Si	0.01382578	0.48182591	-3.69351510
Si	-0.46800013	-0.48182591	3.69351510
O	-0.23472884	0.16410484	-4.44910449
O	-0.39883368	-0.16410484	4.44910449
O	0.16854686	-0.23549744	-4.77230512
O	0.40404430	0.23549744	4.77230512
Si	0.48145647	0.02024770	-5.52598279
Si	0.46120877	-0.02024770	5.52598279
O	0.44210640	0.30060332	-6.12776199

O	0.14150308	-0.30060332	6.12776199
O	-0.45089700	-0.14184255	-6.79880864
O	-0.30905446	0.14184255	6.79880864
Si	-0.49635196	-0.46688435	-7.38718340
Si	-0.02946762	0.46688435	7.38718340
O	-0.16996248	-0.38178663	-8.15599295
O	0.21182415	0.38178663	8.15599295
O	-0.14768275	-0.36116421	8.42945629
O	0.21348146	0.36116421	-8.42945629
H	-0.37023241	-0.43097187	8.41104873
H	0.06073945	0.43097187	-8.41104873
H	0.11724788	0.16297357	8.39891982
H	-0.04572569	-0.16297357	-8.39891982

Hydrogenated surface 36 layers B3LYP/6-31G*
surface vectors

5.00346790 0.00000000
-2.50173400 4.33313030

fractional coordinates

O	0.26642079	0.41242192	-0.23102528
O	-0.14600114	-0.41242192	0.23102528
Si	0.00494550	0.47138847	-0.92090874
Si	-0.46644298	-0.47138847	0.92090874
O	-0.25941139	0.15068908	-1.59662758
O	-0.41010047	-0.15068908	1.59662758
O	0.15772208	-0.26693818	-2.09295510
O	0.42466026	0.26693818	2.09295510
Si	0.47889673	-0.00321682	-2.76826718
Si	0.48211355	0.00321682	2.76826718
O	0.41691307	0.25588276	-3.46386751
O	0.16103030	-0.25588276	3.46386751
O	-0.40306413	-0.15457352	-3.91123886
O	-0.24849061	0.15457352	3.91123886
Si	-0.46316749	-0.47486844	-4.60758489
Si	0.01170096	0.47486844	4.60758489
O	-0.14465784	-0.42528808	-5.27426550
O	0.28063024	0.42528808	5.27426550
O	0.28036072	0.42346016	-5.79673885
O	-0.14309944	-0.42346016	5.79673885
Si	0.02053673	0.48698756	-6.46950369
Si	-0.46645083	-0.48698756	6.46950369
O	-0.22372948	0.17220056	-7.25963858
O	-0.39593004	-0.17220056	7.25963858
O	0.17547171	-0.22276792	-7.51317687
O	0.39823963	0.22276792	7.51317687
Si	0.48439605	0.03129496	-8.29769067
Si	0.45310109	-0.03129496	8.29769067
O	0.44719858	0.31558726	-8.87150021
O	0.13161132	-0.31558726	8.87150021
O	-0.45994082	-0.13324738	-9.59879677

O	-0.32669343	0.13324738	9.59879677
Si	-0.49907305	-0.45908705	-10.15368411
Si	-0.03998599	0.45908705	10.15368411
O	-0.16991263	-0.36787272	-10.92291613
O	0.19796010	0.36787272	10.92291613
O	-0.15528069	-0.35823678	11.15936534
O	0.20295610	0.35823678	-11.15936534
H	-0.37923252	-0.43551489	11.16173165
H	0.05628238	0.43551489	-11.16173165
H	0.10043671	0.14645054	11.11956088
H	-0.04601384	-0.14645054	-11.11956088

Hydrogenated surface 36 layers B3LYP/L
surface vectors

5.01035882 0.00000000
-2.50517941 4.33909802

fractional coordinates

O	0.26102199	0.41251194	-0.22328880
O	-0.15148995	-0.41251194	0.22328880
Si	0.00031368	0.47099264	-0.92068989
Si	-0.47067895	-0.47099264	0.92068989
O	-0.26245011	0.14948186	-1.59530654
O	-0.41193197	-0.14948186	1.59530654
O	0.15427910	-0.26768065	-2.09183791
O	0.42195975	0.26768065	2.09183791
Si	0.47567179	-0.00462446	-2.76508722
Si	0.48029625	0.00462446	2.76508722
O	0.41458510	0.25515674	-3.45583685
O	0.15942836	-0.25515674	3.45583685
O	-0.40813332	-0.15655609	-3.91114505
O	-0.25157722	0.15655609	3.91114505
Si	-0.46811983	-0.47704428	-4.60267317
Si	0.00892445	0.47704428	4.60267317
O	-0.14901987	-0.42454212	-5.27386277
O	0.27552225	0.42454212	5.27386277
O	0.27285816	0.41830736	-5.78103297
O	-0.14544920	-0.41830736	5.78103297
Si	0.01255579	0.48029144	-6.45697632
Si	-0.46773565	-0.48029144	6.45697632
O	-0.23573142	0.16285002	-7.21463903
O	-0.39858144	-0.16285002	7.21463903
O	0.16705960	-0.23651918	-7.53333075
O	0.40357878	0.23651918	7.53333075
Si	0.47993278	0.01871314	-8.28884506
Si	0.46121965	-0.01871314	8.28884506
O	0.44072345	0.29901626	-8.89156193
O	0.14170720	-0.29901626	8.89156193
O	-0.45303856	-0.14389031	-9.56175939
O	-0.30914825	0.14389031	9.56175939
Si	-0.49785146	-0.46858139	-10.15142296

Si	-0.02927007	0.46858139	10.15142296
O	-0.17152937	-0.38351506	-10.92048572
O	0.21198570	0.38351506	10.92048572
O	-0.14708927	-0.35912239	11.19403422
O	0.21203311	0.35912239	-11.19403422
H	-0.36957298	-0.42868674	11.17455991
H	0.05911376	0.42868674	-11.17455991
H	0.11775879	0.16469053	11.16233248
H	-0.04693173	-0.16469053	-11.16233248

Cleaved surface 18 layers PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	20.80000000

fractional coordinates

O	0.70083900	0.08949200	0.83692900
O	0.26599900	0.43199200	0.77439000
O	0.85615600	0.59475000	0.75585100
O	0.61549300	0.87257600	0.68863800
O	0.43864900	0.28526600	0.66633900
O	0.18270700	0.76441400	0.60086400
O	0.76441400	0.18270700	0.57859100
O	0.28526600	0.43864900	0.51311500
O	0.87257600	0.61549300	0.49081600
O	0.59475100	0.85615600	0.42360300
O	0.43199200	0.26599900	0.40506400
O	0.08949200	0.70083900	0.34252400
Si	0.92831300	0.35698600	0.79534900
Si	0.54189900	0.54894800	0.72230700
Si	0.49928300	0.02624300	0.63381200
Si	0.02624300	0.49928300	0.54564200
Si	0.54894900	0.54189800	0.45714700
Si	0.35698600	0.92831300	0.38410600

Cleaved surface 18 layers PW91

cell vectors

5.05617610	0.00000000	0.00000000
-2.52808800	4.37877690	0.00000000
0.00000000	0.00000000	20.80000000

fractional coordinates

O	0.69862600	0.08331700	0.83617600
O	0.26325200	0.43262400	0.77411600
O	0.85271400	0.59306900	0.75671300
O	0.61694700	0.87289300	0.68861200
O	0.44057500	0.28594100	0.66685500
O	0.18934700	0.77042800	0.60007900
O	0.77042800	0.18934700	0.57937600
O	0.28594100	0.44057500	0.51259900
O	0.87289300	0.61694700	0.49084200

O	0.59307000	0.85271400	0.42274100
O	0.43262400	0.26325200	0.40533800
O	0.08331700	0.69862600	0.34327700
Si	0.92422200	0.35255900	0.79492400
Si	0.54091300	0.54946900	0.72267000
Si	0.50353300	0.02957600	0.63400100
Si	0.02957600	0.50353300	0.54545300
Si	0.54947000	0.54091200	0.45678400
Si	0.35255900	0.92422200	0.38453100

Cleaved surface 27 layers PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	26.30000000

fractional coordinates

O	0.69281800	0.08196800	0.98536800
O	0.25730800	0.42237600	0.93546900
O	0.84690600	0.58380000	0.92037800
O	0.60546500	0.86478500	0.86801000
O	0.42925400	0.27818800	0.84958200
O	0.17732100	0.75888900	0.79788200
O	0.76096400	0.17612700	0.78127200
O	0.27041200	0.43285000	0.72700800
O	0.85585300	0.60329100	0.71190600
O	0.60329200	0.85585300	0.65687700
O	0.43285000	0.27041200	0.64177500
O	0.17612700	0.76096400	0.58751000
O	0.75888900	0.17732100	0.57090000
O	0.27818800	0.42925400	0.51920000
O	0.86478500	0.60546400	0.50077200
O	0.58380100	0.84690500	0.44840400
O	0.42237600	0.25730800	0.43331400
O	0.08196800	0.69281800	0.38341400
Si	0.91928600	0.34705900	0.95197200
Si	0.53272700	0.54016500	0.89416200
Si	0.49252500	0.01965200	0.82432500
Si	0.01633700	0.49348900	0.75449100
Si	0.54019300	0.54019300	0.68439100
Si	0.49348900	0.01633600	0.61429100
Si	0.01965200	0.49252500	0.54445800
Si	0.54016600	0.53272700	0.47462000
Si	0.34705900	0.91928500	0.41681000

Cleaved surface 36 layers PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	31.90000000

fractional coordinates

O	0.68419400	0.07348400	0.98768000
O	0.24746700	0.41664500	0.94643500
O	0.83820000	0.57986900	0.93490800
O	0.60042100	0.86380400	0.89158300
O	0.42583600	0.27813100	0.87580400
O	0.17462600	0.75696800	0.83340000
O	0.75865900	0.17384900	0.82002000
O	0.26578000	0.42906300	0.77489600
O	0.85142800	0.59965400	0.76266900
O	0.59958300	0.85133300	0.71707600
O	0.42953700	0.26613400	0.70473400
O	0.17506700	0.75911000	0.65957400
O	0.75911000	0.17506600	0.64654800
O	0.26613400	0.42953700	0.60138800
O	0.85133300	0.59958300	0.58904600
O	0.59965500	0.85142800	0.54345300
O	0.42906300	0.26578000	0.53122700
O	0.17385000	0.75865900	0.48610200
O	0.75696800	0.17462600	0.47272200
O	0.27813100	0.42583600	0.43031800
O	0.86380400	0.60042100	0.41453900
O	0.57986900	0.83820000	0.37121400
O	0.41664500	0.24746600	0.35968700
O	0.07348400	0.68419400	0.31844200
Si	0.90977000	0.34038500	0.96032700
Si	0.52597300	0.53774200	0.91288500
Si	0.48885500	0.01841200	0.85532300
Si	0.01289300	0.49067800	0.79773300
Si	0.53606000	0.53597900	0.73985200
Si	0.49136300	0.01306000	0.68196600
Si	0.01306000	0.49136300	0.62415600
Si	0.53598000	0.53606000	0.56627000
Si	0.49067800	0.01289200	0.50838900
Si	0.01841300	0.48885500	0.45079900
Si	0.53774200	0.52597300	0.39323700
Si	0.34038500	0.90976900	0.34579500

Reconstructed surface 18 layers PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	19.80000000

fractional coordinates

O	0.27546000	0.41465500	0.98743300
O	0.77573800	0.41449500	0.02240900
O	0.77958000	0.11475000	0.90981200
O	0.58018200	0.71406700	0.10010700
O	0.07925400	0.71442800	0.90982200
O	0.28059200	0.11510500	0.10010500
O	0.00322900	0.41461600	0.79334100

O	0.35620200	0.41459800	0.21673800
O	0.82208800	0.82126800	0.80210300
O	0.94382900	0.82109800	0.20765800
O	0.41542800	0.00796300	0.80212900
O	0.53733800	0.00810600	0.20764200
Si	0.97455600	0.41458000	0.95824300
Si	0.47499000	0.41458000	0.05149900
Si	0.75453500	0.08793100	0.82684600
Si	0.60430500	0.74113600	0.18307000
Si	0.08119000	0.74128400	0.82685100
Si	0.27774400	0.08805100	0.18307000

Reconstructed surface 27 layers PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	25.70000000

fractional coordinates

O	0.15607300	0.76539900	0.03099000
O	0.39067300	0.23460100	0.96901000
O	0.75109200	0.17552300	0.04110400
O	0.57556900	0.82447700	0.95889600
O	0.26421000	0.43857200	0.09861400
O	0.82563600	0.56142800	0.90138600
O	0.81937400	0.55025300	0.11878900
O	0.26912100	0.44974700	0.88121100
O	0.59105800	0.78657000	0.18336200
O	0.80448800	0.21343000	0.81663800
O	0.34431100	0.19239100	0.18365600
O	0.15192000	0.80760900	0.81634400
O	0.38994100	0.48264800	0.27331200
O	0.90729400	0.51735200	0.72668800
O	0.97701400	0.88923500	0.26347300
O	0.08777900	0.11076500	0.73652700
O	0.56887000	0.07386900	0.26896800
O	0.49500100	0.92613100	0.73103200
Si	0.46943000	0.00000000	0.00000000
Si	0.99547700	0.48225700	0.07219900
Si	0.51322000	0.51774300	0.92780100
Si	0.50244900	0.49192800	0.14535100
Si	0.01052000	0.50807200	0.85464900
Si	0.63393200	0.81056600	0.24723500
Si	0.82336600	0.18943400	0.75276500
Si	0.31677800	0.15815000	0.24740100
Si	0.15862700	0.84185000	0.75259900

Reconstructed surface 27 layers PW91

cell vectors

5.05617610	0.00000000	0.00000000
-2.52808800	4.37877690	0.00000000

0.00000000 0.00000000 25.70000000
fractional coordinates
O 0.16003000 0.76325900 0.03062400
O 0.39677100 0.23674100 0.96937600
O 0.75309400 0.17487400 0.04137300
O 0.57822000 0.82512600 0.95862700
O 0.25565400 0.43963300 0.10095800
O 0.81601800 0.56036700 0.89904200
O 0.81336200 0.55718900 0.11730900
O 0.25617300 0.44281100 0.88269100
O 0.59274700 0.78961300 0.18461300
O 0.80313400 0.21038700 0.81538700
O 0.35321000 0.19810400 0.18479000
O 0.15510600 0.80189600 0.81521000
O 0.39390600 0.48468800 0.27443500
O 0.90921900 0.51531200 0.72556500
O 0.98000200 0.89382700 0.26406200
O 0.08617500 0.10617300 0.73593800
O 0.56965200 0.07415600 0.27055200
O 0.49549600 0.92584400 0.72944800
Si 0.47353900 0.00000000 0.00000000
Si 0.99368200 0.48375600 0.07228500
Si 0.50992600 0.51624400 0.92771500
Si 0.50228100 0.49643400 0.14625500
Si 0.00584600 0.50356600 0.85374500
Si 0.63550700 0.81263900 0.24848200
Si 0.82286900 0.18736100 0.75151800
Si 0.32133400 0.16106500 0.24845500
Si 0.16026800 0.83893500 0.75154500

Reconstructed surface 36 layers PBE
cell vectors

5.05224940 0.00000000 0.00000000
-2.52612470 4.37537630 0.00000000
0.00000000 0.00000000 31.20000000
fractional coordinates
O 0.83724100 0.59313700 0.00458200
O 0.24410500 0.40686300 0.99541800
O 0.58633100 0.84443100 0.05183300
O 0.74190100 0.15556900 0.94816700
O 0.43844600 0.27095100 0.06686800
O 0.16749600 0.72904900 0.93313200
O 0.19205900 0.77877000 0.11496800
O 0.41328900 0.22123000 0.88503200
O 0.79421300 0.17986900 0.12191800
O 0.61434400 0.82013100 0.87808200
O 0.30999200 0.44604400 0.16815500
O 0.86394800 0.55395600 0.83184500
O 0.85857700 0.54556200 0.18701700
O 0.31301600 0.45443800 0.81298300

O	0.62524900	0.78789800	0.23858500
O	0.83735100	0.21210200	0.76141500
O	0.37279500	0.19255300	0.23876500
O	0.18024200	0.80744700	0.76123500
O	0.41920900	0.48293100	0.31258400
O	0.93627800	0.51706900	0.68741600
O	0.00704400	0.88951100	0.30472800
O	0.11753300	0.11048900	0.69527200
O	0.59910700	0.07472900	0.30892800
O	0.52437800	0.92527100	0.69107200
Si	0.52645400	0.52770300	0.02953100
Si	0.99875100	0.47229700	0.97046900
Si	0.50312800	0.01708900	0.08916100
Si	0.48603900	0.98291100	0.91083900
Si	0.03621600	0.48763300	0.14780200
Si	0.54858200	0.51236700	0.85219800
Si	0.53986300	0.49322100	0.20750700
Si	0.04664100	0.50677900	0.79249300
Si	0.66403300	0.81089900	0.29124500
Si	0.85313400	0.18910100	0.70875500
Si	0.34629900	0.15828200	0.29126700
Si	0.18801600	0.84171800	0.70873300

Hydrogenated surface 18L PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	22.00000000

fractional coordinates

H	0.61665800	0.55777300	0.74517400
H	0.05888400	0.44222700	0.25482600
H	0.11100200	0.16613800	0.74268000
H	0.94486400	0.83386200	0.25732000
O	0.82346100	0.61703600	0.24584200
O	0.20642600	0.38296400	0.75415800
O	0.55259000	0.85645000	0.18204600
O	0.69614000	0.14355000	0.81795400
O	0.44546000	0.29857800	0.15373300
O	0.14688100	0.70142200	0.84626700
O	0.18588500	0.78142200	0.08875100
O	0.40446300	0.21857800	0.91124900
O	0.78401400	0.17998500	0.07877400
O	0.60402900	0.82001500	0.92122600
O	0.27959900	0.42799800	0.01096800
O	0.85160100	0.57200200	0.98903200
O	0.83918700	0.63037700	0.74394100
O	0.20881000	0.36962300	0.25605900
Si	0.50168400	0.53363400	0.20974800
Si	0.96805100	0.46636600	0.79025200
Si	0.49230200	0.02750700	0.12524100

Si	0.46479400	0.97249300	0.87475900
Si	0.02391400	0.49048500	0.04228800
Si	0.53342900	0.50951500	0.95771200

Hydrogenated surface 18L PW91

cell vectors

5.05617610	0.00000000	0.00000000
-2.52808800	4.37877690	0.00000000
0.00000000	0.00000000	22.00000000

fractional coordinates

H	0.60831800	0.55125900	0.74717500
H	0.05705800	0.44874100	0.25282500
H	0.10357200	0.16125700	0.74312800
H	0.94231400	0.83874300	0.25687200
O	0.82103600	0.62193500	0.24553200
O	0.19910200	0.37806500	0.75446800
O	0.55399300	0.86276100	0.18145200
O	0.69123200	0.13723900	0.81854800
O	0.44928700	0.30595100	0.15266200
O	0.14333600	0.69404900	0.84733800
O	0.19461700	0.79040200	0.08729500
O	0.40421500	0.20959800	0.91270500
O	0.79299200	0.18885900	0.07933800
O	0.60413300	0.81114100	0.92066200
O	0.28890000	0.42986300	0.01185900
O	0.85903700	0.57013700	0.98814100
O	0.83131400	0.62677200	0.74646300
O	0.20454200	0.37322800	0.25353700
Si	0.50194400	0.53929700	0.20859600
Si	0.96264800	0.46070300	0.79140400
Si	0.49742700	0.03555900	0.12467400
Si	0.46186700	0.96444100	0.87532600
Si	0.03320800	0.49517300	0.04199500
Si	0.53803500	0.50482700	0.95800500

Hydrogenated surface 27L PBE

cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	27.00000000

fractional coordinates

H	0.93634400	0.37795100	0.68864400
H	0.37795100	0.93634400	0.31135600
H	0.05225100	0.88018500	0.68612200
H	0.88018500	0.05225100	0.31387800
O	0.57456400	0.82503200	0.97304200
O	0.82503200	0.57456400	0.02695800
O	0.40252100	0.23847300	0.95859300
O	0.23847300	0.40252100	0.04140700
O	0.15311600	0.73158200	0.90477500

O	0.73158200	0.15311600	0.09522500
O	0.73207700	0.15132100	0.88953100
O	0.15132100	0.73207700	0.11046900
O	0.22071700	0.39673700	0.83311600
O	0.39673700	0.22071700	0.16688400
O	0.81479000	0.58852100	0.82409500
O	0.58852100	0.81479000	0.17590500
O	0.55634600	0.84478400	0.77031600
O	0.84478400	0.55634600	0.22968400
O	0.44131900	0.29146000	0.74896500
O	0.29146000	0.44131800	0.25103500
O	0.17231700	0.78445600	0.69605300
O	0.78445600	0.17231700	0.30394700
O	0.78432600	0.15610500	0.68696700
O	0.15610500	0.78432600	0.31303300
Si	0.50875000	0.50875000	0.00000000
Si	0.46644500	0.98694100	0.93157300
Si	0.98694100	0.46644500	0.06842700
Si	0.98113000	0.46818000	0.86266100
Si	0.46818000	0.98113000	0.13733900
Si	0.50836500	0.52891800	0.79453100
Si	0.52891800	0.50836500	0.20546900
Si	0.49450300	0.02352500	0.72533500
Si	0.02352500	0.49450300	0.27466500

Hydrogenated surface 36L PBE
cell vectors

5.05224940	0.00000000	0.00000000
-2.52612470	4.37537630	0.00000000
0.00000000	0.00000000	32.00000000

fractional coordinates

H	0.61102600	0.55266800	0.34754600
H	0.05835800	0.44733200	0.65245400
H	0.10738900	0.16375300	0.34961900
H	0.94363700	0.83624700	0.65038100
O	0.26405700	0.41600500	0.99321700
O	0.84805300	0.58399500	0.00678300
O	0.75573300	0.16531500	0.94860100
O	0.59041900	0.83468500	0.05139900
O	0.17076200	0.75022700	0.93634900
O	0.42053600	0.24977300	0.06365100
O	0.41996400	0.25583400	0.89139600
O	0.16413000	0.74416600	0.10860400
O	0.59360200	0.84239300	0.87853500
O	0.75120900	0.15760700	0.12146500
O	0.84826600	0.58214400	0.83471000
O	0.26612200	0.41785600	0.16529000
O	0.27062500	0.42541900	0.82027700
O	0.84520500	0.57458100	0.17972300
O	0.77730200	0.18210900	0.77383400

O	0.59519400	0.81789100	0.22616600
O	0.18185900	0.78160200	0.76622700
O	0.40025700	0.21839800	0.23377300
O	0.44211000	0.29927300	0.72153100
O	0.14283700	0.70072700	0.27846900
O	0.55370600	0.85927400	0.70269700
O	0.69443200	0.14072600	0.29730300
O	0.82314900	0.62002800	0.65858100
O	0.20312000	0.37997200	0.34141900
O	0.83339300	0.62461100	0.34861000
O	0.20878200	0.37538900	0.65139000
Si	0.00975600	0.47953200	0.97126200
Si	0.53022400	0.52046800	0.02873800
Si	0.48555300	0.00358500	0.91366800
Si	0.48196800	0.99641500	0.08633200
Si	0.53239200	0.52620700	0.85632200
Si	0.00618500	0.47379300	0.14367800
Si	0.01862500	0.49344400	0.79856200
Si	0.52518100	0.50655600	0.20143800
Si	0.48876800	0.02915900	0.74142500
Si	0.45961000	0.97084100	0.25857500
Si	0.50116700	0.53686500	0.68329400
Si	0.96430300	0.46313500	0.31670600

CO adsorbed B3LYP/L

surface vectors

10.02071764 0.00000000
-5.01035882 8.67819604

fractional coordinates

Si	-0.22802290	0.26526238	-0.92659805
Si	-0.49328528	-0.26526238	0.92659805
Si	0.26059831	-0.25085314	-0.91392785
Si	-0.48854855	0.25085314	0.91392785
Si	0.26895063	0.26246239	-0.94795466
Si	0.00648824	-0.26246239	0.94795466
Si	-0.23657802	-0.24927093	-0.93267569
Si	0.01269291	0.24927093	0.93267569
Si	0.22411110	0.48673967	-2.82692163
Si	-0.26262857	-0.48673967	2.82692163
Si	-0.26992502	-0.01313035	-2.68045101
Si	-0.25679467	0.01313035	2.68045101
Si	-0.26431745	0.49094766	-2.82567131
Si	0.24473489	-0.49094766	2.82567131
Si	0.22824273	-0.01358983	-2.70191203
Si	0.24183257	0.01358983	2.70191203
Si	-0.01170663	-0.25863309	-4.63778871
Si	0.24692646	0.25863309	4.63778871
Si	0.48351997	0.22670589	-4.62521637
Si	0.25681409	-0.22670589	4.62521637
Si	0.48568410	-0.26110321	-4.57973556

Si	-0.25321269	0.26110321	4.57973556
Si	-0.02073936	0.22031168	-4.65315447
Si	-0.24105104	-0.22031168	4.65315447
O	0.11077067	-0.30979007	5.66088525
O	0.42056074	0.30979007	-5.66088525
O	-0.39934075	0.16651155	5.60665236
O	0.43414769	-0.16651155	-5.60665236
O	-0.37486315	-0.28223513	5.79601302
O	-0.09262802	0.28223513	-5.79601302
O	0.10018757	0.17827698	5.67408532
O	-0.07808942	-0.17827698	-5.67408532
O	-0.06564949	0.29875624	-0.25796274
O	-0.36440573	-0.29875624	0.25796274
O	0.42106322	-0.22589707	-0.27198843
O	-0.35303971	0.22589707	0.27198843
O	0.43238363	0.29578740	-0.30465404
O	0.13659623	-0.29578740	0.30465404
O	-0.07764752	-0.22577474	-0.27658517
O	0.14812722	0.22577474	0.27658517
O	-0.19367903	0.42053207	-1.74149356
O	0.38578890	-0.42053207	1.74149356
O	0.29529993	-0.09062583	-1.64696940
O	0.38592576	0.09062583	1.64696940
O	0.29811516	0.41381639	-1.79934899
O	-0.11570123	-0.41381639	1.79934899
O	-0.20172363	-0.08635638	-1.60345258
O	-0.11536725	0.08635638	1.60345258
O	0.19228728	-0.39079368	-2.00985040
O	-0.41691904	0.39079368	2.00985040
O	-0.29550175	0.11759604	-1.94238571
O	-0.41309779	-0.11759604	1.94238571
O	-0.29847285	-0.38426161	-2.07382588
O	0.08578876	0.38426161	2.07382588
O	0.19858764	0.11217897	-1.92838947
O	0.08640867	-0.11217897	1.92838947
O	0.06597618	0.34903923	-3.47487885
O	-0.28306305	-0.34903923	3.47487885
O	-0.43166834	-0.15209939	-3.27536194
O	-0.27956894	0.15209939	3.27536194
O	-0.42259800	0.34961920	-3.43038779
O	0.22778280	-0.34961920	3.43038779
O	0.06722682	-0.14921078	-3.33059124
O	0.21643760	0.14921078	3.33059124
O	-0.14788704	-0.42578405	-4.08866368
O	0.27789701	0.42578405	4.08866368
O	0.34591345	0.06880182	-3.95149849
O	0.27711163	-0.06880182	3.95149849
O	0.34095169	-0.42429489	-4.07238922
O	-0.23475343	0.42429489	4.07238922
O	-0.15409274	0.06178618	-3.94971557

O	-0.21587891	-0.06178618	3.94971557
O	0.12199326	-0.27806457	-5.43469901
O	0.40005783	0.27806457	5.43469901
O	-0.40337221	0.17602922	-5.41368126
O	0.42059858	-0.17602922	5.41368126
O	-0.39541577	-0.30455510	-5.37058632
O	-0.09086067	0.30455510	5.37058632
O	0.10311007	0.17793460	-5.36391749
O	-0.07482454	-0.17793460	5.36391749
H	-0.02759254	0.41463532	5.58060072
H	-0.44222787	-0.41463532	-5.58060072
H	0.48373399	-0.06401599	5.57353426
H	-0.45225002	0.06401599	-5.57353426
H	0.43310103	0.34529039	6.23140868
H	0.08781064	-0.34529039	-6.23140868
H	-0.01458539	-0.06889242	5.62966501
H	0.05430702	0.06889242	-5.62966501
H	0.03655478	-0.27208416	5.63289825
H	0.30863894	0.27208416	-5.63289825
H	-0.48139706	0.19403740	5.53955385
H	0.32456554	-0.19403740	-5.53955385
H	-0.45623256	-0.25474832	5.68833375
H	-0.20148425	0.25474832	-5.68833375
H	0.02333437	0.21232403	5.59975160
H	-0.18898967	-0.21232403	-5.59975160
C	-0.47909129	0.47299597	7.88182628
C	0.04791274	-0.47299597	-7.88182628
O	-0.42687826	-0.45811024	8.82454261
O	0.03123198	0.45811024	-8.82454261

CO adsorbed PBE
cell vectors

10.10449880	0.00000000	0.00000000
-5.05224940	8.75075260	0.00000000
0.00000000	0.00000000	22.00000000

fractional coordinates

H	0.41966400	0.33430300	0.28429600
H	0.54387500	0.75274300	0.25661100
H	0.79359000	0.25102300	0.74303400
H	0.51119100	0.19257600	0.25146300
H	0.31477800	0.79660000	0.74736600
H	0.04119700	0.74503500	0.25739300
H	0.29236700	0.24923200	0.74326300
H	0.01071400	0.19707800	0.25301100
H	0.81640800	0.79987700	0.74892900
H	0.06632500	0.60797000	0.73793100
H	0.48070100	0.93635800	0.25541200
H	0.54445700	0.06119700	0.74436800
H	0.95717400	0.38915600	0.26169500
H	0.57067200	0.61283600	0.73734000

H	0.98264300	0.93587600	0.25682100
H	0.04332700	0.05981800	0.74599000
C	0.49968100	0.47534700	0.35716100
O	0.54570700	0.55591900	0.39829700
O	0.38664000	0.26338000	0.24930900
O	0.61511900	0.71569500	0.75455300
O	0.89718200	0.28439700	0.24641500
O	0.59539700	0.17161900	0.75397700
O	0.42160200	0.82543000	0.24644000
O	0.11185000	0.71206200	0.75401100
O	0.09439700	0.17105100	0.75430200
O	0.92415900	0.82574800	0.24640100
O	0.35393400	0.58081000	0.81561400
O	0.76814300	0.41588300	0.18527000
O	0.35369800	0.06760900	0.82458700
O	0.28053600	0.92355400	0.17503800
O	0.85148500	0.58028800	0.81550500
O	0.27037500	0.41117500	0.18666100
O	0.85325800	0.07011700	0.82503600
O	0.78856900	0.93207500	0.17572200
O	0.57604100	0.35499400	0.83814700
O	0.22024900	0.63670000	0.16337800
O	0.57146200	0.85832900	0.84921400
O	0.71353400	0.14047600	0.15112500
O	0.07706600	0.35701800	0.83796900
O	0.71945700	0.64305600	0.16276500
O	0.07343000	0.85405700	0.85015600
O	0.21034000	0.13644800	0.15198500
O	0.69316500	0.60638600	0.90707800
O	0.08787800	0.38688600	0.09411100
O	0.70351500	0.11159900	0.91639800
O	0.58928700	0.88268200	0.08680200
O	0.19660600	0.60718900	0.90732300
O	0.58551500	0.39148400	0.09350600
O	0.20389200	0.10956600	0.91569300
O	0.09019300	0.88579600	0.08397400
O	0.29928400	0.40984200	0.91631400
O	0.88569000	0.58562800	0.08428600
O	0.29491300	0.90382300	0.92732000
O	0.38685400	0.09385000	0.07440000
O	0.79890900	0.41161100	0.91677200
O	0.38788000	0.58185900	0.08515200
O	0.79104300	0.90320100	0.92677800
O	0.88433400	0.09196900	0.07259900
O	0.42933600	0.30285000	0.98965100
O	0.12330500	0.69192900	0.01077600
O	0.40992800	0.76391300	0.99124400
O	0.64362600	0.23154400	0.01155600
O	0.93070300	0.30567500	0.98989600
O	0.62495800	0.69320400	0.01151700

O	0.91024300	0.76504600	0.98916400
O	0.14180900	0.22853700	0.01037500
O	0.62379900	0.72375800	0.26248300
O	0.90416000	0.28510800	0.73910700
O	0.59209800	0.16380200	0.25507600
O	0.42543100	0.82999300	0.74497600
O	0.11658900	0.70944700	0.26120500
O	0.40272500	0.28259200	0.73900400
O	0.08727900	0.16287700	0.25630800
O	0.92731400	0.83383600	0.74713600
Si	0.48882200	0.74638700	0.79136200
Si	0.73982100	0.25089800	0.20927400
Si	0.47981700	0.22056800	0.78823000
Si	0.25632000	0.77268400	0.21212800
Si	0.98858500	0.74526600	0.79181000
Si	0.23690300	0.24427000	0.21106700
Si	0.98017700	0.22193800	0.78839200
Si	0.75994200	0.77888900	0.21234500
Si	0.72996200	0.48806300	0.87012100
Si	0.24234200	0.50392700	0.13183700
Si	0.73136800	0.98750000	0.87983900
Si	0.74366600	0.01040900	0.12108500
Si	0.23177800	0.48834700	0.87002100
Si	0.73993400	0.50950800	0.13094200
Si	0.23324300	0.98550900	0.87990300
Si	0.24196200	0.00849400	0.12096000
Si	0.26792400	0.26268200	0.95765200
Si	0.00148900	0.73177400	0.04249700
Si	0.25536300	0.74155300	0.95886900
Si	0.51078800	0.25515900	0.04270100
Si	0.76851900	0.26506100	0.95831800
Si	0.50228000	0.73046100	0.04415900
Si	0.75379600	0.74180600	0.95833800
Si	0.01078400	0.25382500	0.04211700