

Tetrahedral honeycomb surface reconstructions of quartz, cristobalite and stishovite

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Supplementary information

1. Initial substrates for evolutionary search

Structure	Composition (Si-O)	Cell shape (a,b,c in Å)	Cell shape (α,β,γ)
O-terminated α -quartz (001)	3 - 6	4.91, 4.91, 4.89	90°, 90°, 120°
O-terminated α -cristobalite (001)	4 - 6	4.98, 4.98, 6.45	90°, 90°, 90°
Si-terminated stishovite (100)	4 - 6	4.18, 2.67, 8.35	90°, 90°, 90°
O-terminated stishovite (110)	4 - 6	2.67, 5.91, 5.24	90°, 90°, 90°

Here, c means the thickness of the substrate in the direction perpendicular to the slab

2. POSCAR files of discussed surfaces

Dense cristobalite

```
1.0000000000000000
 9.955999999999995 0.0000000000000000 0.0000000000000000
 0.0000000000000000 4.977999999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 41.398800000000014
Si O
28 56
Direct
0.1613091805894626 0.2188405858909590 0.3703307939771889
0.6612512718107766 0.2343835090263653 0.3693379400635024
0.1946694945627669 0.7187382922252894 0.3265755575132090
0.6971414103956022 0.7383365256453800 0.3257391559042233
0.4433803734795205 0.7664996022601471 0.2824910021939004
```

0.9468812196948093 0.5718134309986311 0.2826586133309661
0.4394974460421324 0.2676954555589504 0.2390537195792746
0.9419582899688166 0.0716695821793465 0.2388442121185648
0.0900566221762773 0.9802951977359839 0.6051142356134704
0.5772398271830426 0.4999648389997375 0.0898618965477098
0.5898179173298104 0.4301044410620705 0.6054103973382894
0.0772268398979605 0.9476087476365933 0.0898658239459209
0.2766897166282689 0.4390848035730528 0.6054619810753366
0.7638598220566095 0.9587281894687081 0.0896273833923829
0.7765009794120772 0.9713922567640623 0.6052634903227272
0.2638641439901903 0.4888820713283764 0.0897240561837620
0.1993584099971315 0.7040051258815083 0.4999392494807395
0.6900074703304924 0.2210435252363681 0.1951369405761199
0.4138265403482038 0.0651406336120317 0.4119451744192943
0.1849932789349609 0.2096724754644725 0.5434748767286450
0.6721312081586959 0.7282796625094150 0.1515608851993164
0.4489438374365449 0.5624907897808740 0.4552144008442340
0.6953596500015848 0.7097329877983398 0.5000345492117475
0.1901235335000280 0.2300497130732921 0.1950162868940168
0.9101985987674510 0.2545646430684911 0.4139908750617067
0.6815522745078155 0.1991373493337321 0.5435373816206877
0.1729878604186865 0.7228068253395676 0.1515680081029060
0.9452148754119918 0.7548738657751670 0.4571608832806859
0.1848396067814662 0.7117158425311274 0.6076304682661089
0.6722625631184656 0.2316933508898771 0.0874605855046795
0.6823258952443041 0.1989608750795782 0.6237885722162773
0.1695087960500388 0.7168566617458225 0.0713370848481958
0.6847766146685359 0.6986530454159663 0.6077170561236969
0.1720549644097176 0.2162456052260708 0.0875081320616431
0.1819972300954831 0.2110159952044341 0.6237179959916404
0.6691016084861019 0.7311624760474942 0.0712787490314142
0.4335597455375364 0.4714854983842400 0.6190791316646127
0.9211001998011241 0.9902144502011723 0.0761931123650470
0.9336881930865815 0.9386290550204777 0.6186093895868368
0.4210493973310392 0.4567922813285392 0.0762731720388672
0.1317882985663061 0.4551661441846377 0.5204229335519983
0.6203473304930753 0.9722100671049105 0.1750479499628170
0.4478684996395117 0.2526864556685453 0.4429791724531995
0.2957567520003366 0.3449484430720986 0.5677092721493651
0.7827518499714330 0.8650622118126634 0.1274044664437000
0.3339703721248100 0.5949688233204071 0.4825019658749454
0.8270441907729946 0.1160055915400733 0.2117994264409901
0.2436939033025425 0.9622601645183195 0.5218997189128274
0.7305500150174211 0.4792714287761086 0.1728467175673885
0.4234287040293694 0.7542419312805393 0.4239010698700696
0.0924711898852593 0.8048450956741391 0.4728826340335885
0.5859925669831014 0.3191493526362805 0.2229496057732518
0.0714016985502397 0.0775317027624922 0.5673346541433091
0.5583287810246915 0.5983858591553997 0.1275997554298556
0.7367388241171113 0.4446582832043120 0.5211765509701962
0.2321559264423030 0.9755717609816301 0.1721256774878270
0.9304174153459570 0.4439517428035202 0.4456028863895938
0.7944611318197232 0.0661905273334398 0.5674576757934489
0.2827569084123454 0.5828691931934387 0.1274830794146666
0.8326661529166728 0.8276242877066622 0.4842338216962645

0.3258005705309728	0.3406173870450928	0.2123178072422576
0.6258789699537317	0.9518360016079299	0.5211680976164246
0.1208978412807724	0.4822500406975507	0.1755084909462354
0.9266196126928250	0.9439045635449475	0.4254575939822445
0.5938113828359946	0.6239609974362637	0.4712636648870401
0.0873396967213864	0.1236769732457077	0.2224840306563536
0.5699595716465709	0.3328758177889597	0.5677205390675581
0.0582405020810270	0.8492576885512406	0.1275971173519252
0.2630001750359270	0.1218893959294221	0.3987410878919775
0.7609914185574880	0.3067844878526316	0.3992664725247366
0.0215402893052001	0.3220208473466641	0.3864182271497967
0.5191863528402436	0.1210323954976289	0.3828228204275916
0.2277913401393477	0.4694812940694106	0.3508035449885156
0.6318714437171593	0.5035231405718363	0.3481990224329365
0.1277634853727037	0.9686644356123537	0.3462179684732689
0.7307661191556249	0.0035998286857151	0.3471295563955223
0.3335723253964247	0.8275842771886559	0.3105704966913194
0.8365830590619439	0.6334027304802134	0.3103099980168125
0.0951623324654420	0.6144222723170003	0.2981206245901618
0.5928493587422281	0.8181792004069592	0.2970270368183137
0.4256362209534288	0.4573273775533764	0.2707752591331172
0.9260521063123051	0.2638099363351856	0.2704922786362189
0.4219348190862817	0.9588013533614230	0.2511331020452729
0.9305206752854573	0.7625877112885604	0.2510529074554810

Dense surface, α -quartz (001)

1.0000000000000000

9.8260002136230469	0.0000000000000000	0.0000000000000000
-4.9130001068115234	8.5095663070678711	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.7028007507324219

Si O

36 72

Direct

0.2470896418506072	0.2469729961354545	0.2944204633681764
0.2637552302837634	0.0074667135386406	0.2368698565797160
0.4211023803476195	0.3144308998666361	0.5450962036049276
0.0937025846573647	0.1462154284354540	0.5444279332955162
0.2612540437250246	0.2615775955003627	0.4650548292034742
0.0081786469899399	0.4820392685375054	0.3510525093887793
0.2734273459157919	0.0160465670643077	0.4077009417161577
0.1047970498283064	0.4024776943039328	0.1565889340703421
0.4320481306198900	0.0612622776140412	0.1574090123695839
0.7470896269494460	0.2469729961354545	0.2944204633681764
0.7637552302837705	0.0074667135386406	0.2368698565797160
0.9211023803476195	0.3144308998666361	0.5450962036049276
0.5937026070091065	0.1462154284354540	0.5444279332955162
0.7612539841203798	0.2615775955003627	0.4650548292034742
0.5081786665477139	0.4820392685375054	0.3510525093887793
0.7734273459157919	0.0160465670643077	0.4077009417161577
0.6047970349271452	0.4024776943039328	0.1565889340703421
0.9320481008175676	0.0612622776140412	0.1574090123695839
0.2470896716529296	0.7469730408389381	0.2944204633681764
0.2637552600860857	0.5074667824565111	0.2368698565797160
0.4211023803476195	0.8144308998666361	0.5450962036049276
0.0937026070091065	0.6462154433366152	0.5444279332955162
0.2612540735273470	0.7615776551050075	0.4650548292034742
0.0081786930904073	0.9820393877467950	0.3510525093887793
0.2734273459157919	0.5160465735835658	0.4077009417161577

0.1047970796306288 0.9024777539085775 0.1565889340703421
0.4320481306198900 0.5612623074163636 0.1574090123695839
0.7470896865540908 0.7469730408389381 0.2944204633681764
0.7637552302837705 0.5074667824565111 0.2368698565797160
0.9211023803476195 0.8144308998666361 0.5450962036049276
0.5937026070091065 0.6462154433366152 0.5444279332955162
0.7612540437250246 0.7615776551050075 0.4650548292034742
0.5081787261523587 0.9820393877467950 0.3510525093887793
0.7734273459157919 0.5160465735835658 0.4077009417161577
0.6047970945317900 0.9024777539085775 0.1565889340703421
0.9320481604222124 0.5612623074163636 0.1574090123695839
0.4486885918476915 0.1705229943774924 0.5575978736374338
0.0632217713051375 0.4788053534400660 0.5619881283985322
0.2557606054234185 0.2825998019895621 0.5648278550831876
0.4134960858322998 0.3268926945841812 0.4952379919658512
0.2338087628517940 0.3987347672418764 0.4463910013520476
0.3793153468172221 0.3165292358892557 0.3303839107217144
0.4339453432186957 0.0458187391906506 0.3855459013661502
0.1359031432159625 0.4471319595596412 0.3731281707608858
0.1101570180245375 0.1521467178045199 0.4942676117848919
0.2899640386500408 0.1768777799798329 0.4261298985956685
0.0839525408732271 0.1142267552999741 0.3150999337455787
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0.2936330619485830 0.1714491122686326 0.2565738203715711
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0.4149705038550024 0.0499730242474783 0.2075766566817450
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0.2702613546152079 0.0356607680897127 0.1368480492794291
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0.9486885918476915 0.1705229943774924 0.5575978736374338
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0.7899640088477184 0.1768777799798329 0.4261298985956685
0.5839525408732271 0.1142267552999741 0.3150999337455787
0.7316232312129642 0.3906435615351995 0.2751889461228458
0.7936330619485830 0.1714491122686326 0.2565738203715711
0.6121406365809250 0.4234587662818896 0.2064065813051172
0.9149704442503506 0.0499730242474783 0.2075766566817450
0.5771627951847123 0.2307476877623955 0.1443420164976956
0.7702613546152079 0.0356607680897127 0.1368480492794291
0.9627842743192758 0.4247263987266265 0.1396487016049974
0.4486885918476915 0.6705230539821372 0.5575978736374338
0.0632217750304278 0.9788053534400660 0.5619881283985322
0.2557606352257409 0.7825998913965293 0.5648278550831876
0.4134961156346222 0.8268927839911484 0.4952379919658512
0.2338087777529552 0.8987348268465212 0.4463910013520476
0.3793153468172221 0.8165292656915781 0.3303839107217144
0.4339453432186957 0.5458187801688439 0.3855459013661502
0.1359031879194461 0.9471319893619636 0.3731281707608858
0.1101570254751181 0.6521467625080035 0.4942676117848919
0.2899640386500408 0.6768777799798329 0.4261298985956685
0.0839525557743883 0.6142267702011353 0.3150999337455787
0.2316231865094807 0.8906435615351995 0.2751889461228458
0.2936330619485830 0.6714491867744385 0.2565738203715711
0.1121406663832474 0.9234588258865344 0.2064065813051172
0.4149705336573248 0.5499730689509690 0.2075766566817450
0.0771628249870346 0.7307477175647179 0.1443420164976956

0.2702613844175303	0.5356608202437769	0.1368480492794291
0.4627843041215982	0.9247264285289489	0.1396487016049974
0.9486886514523363	0.6705230539821372	0.5575978736374338
0.5632217750304278	0.9788053534400660	0.5619881283985322
0.7557606203245868	0.7825998913965293	0.5648278550831876
0.9134960858322998	0.8268927839911484	0.4952379919658512
0.7338087777529552	0.8987348268465212	0.4463910013520476
0.8793153468172221	0.8165292656915781	0.3303839107217144
0.9339453730210181	0.5458187801688439	0.3855459013661502
0.6359031730182849	0.9471319893619636	0.3731281707608858
0.6101570403762793	0.6521467625080035	0.4942676117848919
0.7899640088477184	0.6768777799798329	0.4261298985956685
0.5839525408732271	0.6142267702011353	0.3150999337455787
0.7316231716083195	0.8906435615351995	0.2751889461228458
0.7936331215532277	0.6714491867744385	0.2565738203715711
0.6121406961855698	0.9234588258865344	0.2064065813051172
0.9149705634596401	0.5499730689509690	0.2075766566817450
0.5771628547893570	0.7307477175647179	0.1443420164976956
0.7702614142198527	0.5356608202437769	0.1368480492794291
0.9627843339239206	0.9247264285289489	0.1396487016049974

Shifted surface, α -quartz (001)

1.00000000000000

9.8260002136230469	0.0000000000000000	0.0000000000000000
-4.9130001068115234	8.5095663070678711	0.0000000000000000
0.0000000000000000	0.0000000000000000	38.2974014282226563

Si O

36 72

Direct

0.2262130943202507	0.2219364318211916	0.3755403707956333
0.2220995696963044	0.7095002116278124	0.3663061481017422
0.2601059166297262	0.4690096686228031	0.3226347004805064
0.1991281248193673	0.9670208517161569	0.3212735442750940
0.2707174059439410	0.2088400178021104	0.5159450669652585
0.2006781444716452	0.7113411605862865	0.5169467256402811
0.4946220775260031	0.4507354263609002	0.4216778905594794
0.4907048739910636	0.9468088638125067	0.4160176530508721
0.2548424619196652	0.4701218590027239	0.4714094371320527
0.2446127090219434	0.9552349872979207	0.4636194648433758
0.4543672962972707	0.2839456279688619	0.5830490982457377
0.4507478799880857	0.5310651343885056	0.2578291803124486
0.3481490125905466	0.7924092591625609	0.5857761530930290
0.3470093859270591	0.0317885119481431	0.2509995891320855
0.1251876219108183	0.1082803490942226	0.5845258397648934
0.1197350566622788	0.3585569056236011	0.2542324450088742
0.0186868716465725	0.6126475706825119	0.5841630677065623
0.0187511397582512	0.8703300098186944	0.2542567277856875
0.7262130943202507	0.2219364318211916	0.3755403707956333
0.7220995845974656	0.7095002116278124	0.3663061481017422
0.7601059166297262	0.4690096686228031	0.3226347004805064
0.6991281546216896	0.9670208517161569	0.3212735442750940
0.7707174357462634	0.2088400178021104	0.5159450669652585
0.7006781593727993	0.7113411605862865	0.5169467256402811
0.9946220477236807	0.4507354263609002	0.4216778905594794
0.9907048739910636	0.9468088638125067	0.4160176530508721
0.7548424619196652	0.4701218590027239	0.4714094371320527
0.7446127388242658	0.9552349872979207	0.4636194648433758
0.9543673260995931	0.2839456279688619	0.5830490982457377
0.9507478501857634	0.5310651343885056	0.2578291803124486
0.8481490423928761	0.7924092591625609	0.5857761530930290
0.8470094157293815	0.0317885119481431	0.2509995891320855

0.6251875921084959 0.1082803490942226 0.5845258397648934
0.6197350715634400 0.3585569056236011 0.2542324450088742
0.5186868809597982 0.6126475706825119 0.5841630677065623
0.5187511174065094 0.8703300098186944 0.2542567277856875
0.2319159206201817 0.3387062174131685 0.5000847588524238
0.1555902282490536 0.8159486871944424 0.4920121592961806
0.3666630111481766 0.2831354126659207 0.4042755667209477
0.3783012361540585 0.8014492439097154 0.3906518141263362
0.4143017711854284 0.5193361628667645 0.4488426872944515
0.4025488930466565 0.9568683426781419 0.4508203164813196
0.1123232242820293 0.4095710368362120 0.4431822501946598
0.1349145991258638 0.9231015238307236 0.4293213748086728
0.1278303851910749 0.0904634877265025 0.5418633718182804
0.1175467718392227 0.3477945572558667 0.2969996837912632
0.0463535561761006 0.6095029520563031 0.5417928652595734
0.0406433701322584 0.8967604065678856 0.2968710737827180
0.2921395494612611 0.1205426229884381 0.4825031915066376
0.2579903473084002 0.6136557334308321 0.4929442109615039
0.1792660163145712 0.7513628567201991 0.6023299866816814
0.1810502607202693 0.0024126719181581 0.2355028502139476
0.3751584566830175 0.6437331313977026 0.5926845973936636
0.3764925513217179 0.8900958615970893 0.2388697844161243
0.2930578184410422 0.1424926612339164 0.6002849564338533
0.2895179622519350 0.3947572452077637 0.2395138850936362
0.4828832616712546 0.4462765998289697 0.6003663463689719
0.4874006004030988 0.6993133984426478 0.2433267314258671
0.4880390143712177 0.9511097468682550 0.6027550237195811
0.4853658363668814 0.1985983677964143 0.2368592142913712
0.4291825089052139 0.2837909211331819 0.5404681797215929
0.4230627656565886 0.5204504450257517 0.3006010247601338
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0.8783012361540585 0.8014492439097154 0.3906518141263362
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0.9025488930466636 0.9568683426781419 0.4508203164813196
0.6123232242820293 0.4095710368362120 0.4431822501946598
0.6349146214776056 0.9231015238307236 0.4293213748086728
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Stable stishovite (100)

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Si O

39 78

Direct

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0.7160478210078622	0.1572155814848557	0.1205462728486140
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0.7151569372695974	0.4905183561258326	0.1991933430183153
0.7151569372695974	0.1571853561258365	0.1991933430183153
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0.2150521369229992	0.3238480492072782	0.2090347158001293
0.2150521369229992	0.9905140492072775	0.2090347158001293
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0.6121174483125884	0.3238419157966845	0.2385368464454771
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Dense stishovite (110)

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Si O

38 76

Direct

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0.4007709435196672	0.3012803386168156	0.3916546333521786
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0.0666777227107470	0.8012232311789369	0.3083997043385424
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0.2363513849577772	0.3012234448435988	0.3095113143440826
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0.5666200659817922	0.3012531510073685	0.3074439200441040
0.8969589381748007	0.3012028581810652	0.4737864815358118
0.8969633049835433	0.3011892310380309	0.3095358124999815
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0.8702825427553409	0.3016203247143744	0.1450228326155805
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0.2341109030050686	0.4949956618539096	0.3916586087812780
0.5665902987091278	0.4951358672732931	0.3916457320314822
0.8991812635281921	0.4949765677223325	0.3916599378401815