

Reconstruction and stability of β -cristobalite 001, 101, and 111 surfaces during dehydroxylation: Supporting Information

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Data content: coordinates for the periodic structures 001-1 to 8, 101-1 to 4 and 111-1 to 4 in the VASP format, and values of the vibrational frequencies for 001-1, 001-2 and H₂O as obtained from VASP calculations.

001-1

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001-2

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001-3

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Si O H

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101-1

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101-3

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101-4

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111-3

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.1350479121969355	.3173533824930770	.6186724747646408
.2548040822444461	.2608163013851013	.5443312387472056
.2480783873826657	.4951865644957604	.5077661814516385
.3292588853370841	.2493405732671813	.6126808848832745
.1642532483648871	.2306824441711469	.5152998182133036
.2229105290602478	.5805556032076363	.6163844986791835
.3381179494919236	.9392051097636381	.2130715132919972
.0835051726540963	.0114556759653977	.5687632949076438
.3319952536771833	.2628098316249118	.4842105384895731
.0757567432295680	.2380885073459662	.5185773798028052
.0775218191791294	.5043021303218862	.5181783931395647
.0282648192725859	.1576820711693522	.3192834217274029
.0314023736075584	.3064313144073048	.4259708754380840
.9976794421664735	.7407194509676380	.5653574491270154
.0247765370166747	.9064688012800349	.3593707432305656
.0868975172255286	.7487605976089401	.5747395727634299
.0590966703059026	.8268864192052506	.4626925569736375
.1904825229608034	.1587838779016739	.3058157288598766
.1297105750346398	.9311616947916944	.2260765323408360
.1352947760904304	.5844373497642406	.6194414298015591
.2585229305512478	.0150158761443868	.5445208175458309
.2757508213155413	.4160099467070870	.3093089078765925
.5243579611294317	.6604855514490582	.3529762547620408
.3612505946935451	.4248465330227803	.2848120140786872
.4434222925360541	.9174091529961644	.3626177613227500
.3602940694306928	.6603418335498935	.3418904538194687
.5285278687786223	.9229331156463619	.3636187954970022
.4490841754030325	.4413313082867993	.2793937117609093
.3332245401295917	.5885640637069576	.2146154414326465
.5262724266275827	.4170376494267087	.3126369190868743
.5371763482211497	.6288695079451542	.2265988046456996
.5860900732045610	.7459732319133253	.5757966967659927
.5603389921526609	.8272659058340189	.4634943216531245
.4973100496608452	.7399234943794637	.5643350903337422
.6118643038234951	.9124479493577409	.3533888426731008
.5319206286126029	.3053955771342365	.4272017346165720
.4165567721268288	.2445755785135408	.6185486182663316
.5759089845537233	.2372010729820986	.5201732838129366
.5780177551488147	.5035908025171665	.5191875099275509
.6349961960921146	.3158898507620160	.6203984700254732
.4925477771296747	.2496788659535998	.5479598853702656
.6351618633863187	.5841305234498899	.6209979341480100
.6330389992774850	.9502011004976658	.2233524187849923
.4060903654634634	.9946131833509141	.5566683329389582
.6644966719353049	.2291465866001348	.5179407420331329
.4131703424114010	.2380172986207321	.4909323088102198

.4212420113176593	.5160766696939596	.4946592261292310
.3661024921298511	.1718994224463847	.2870287240027191
.3974693971636764	.3569459572674235	.3879630976774356
.3219089937531474	.7272810096746620	.5683682308554505
.3607324568102579	.9222337493611464	.3408454907265538
.4095100399549377	.7318322783340410	.5566367901443631
.3723799692026517	.8094857832485308	.4535672484413204
.5261953097889618	.1603885124117788	.3185008339180786
.4823447756662643	.9108316831761181	.2479154352241344
.4162670395150261	.5087927972773786	.6217690135305657
.5832726963855619	.0100229639858326	.5700858616097182
.6090520738584768	.4177594832476502	.3433170891261132
.8607469438858639	.6645067308646234	.3373886823822728
.6923168245642188	.4086986172190179	.3441752387906114
.7782341058472267	.9286306316704360	.3143448219808208
.6972784975806741	.6697313723615645	.3429748954769497
.8599703901863601	.9232192254006909	.3415963820733694
.7761299144391017	.4145895023714573	.3122658330687559
.6623527618666256	.4935574797227145	.2350230349871391
.8606279086323816	.4222784396477874	.2849399589876371
.8351478584359256	.5889316364113761	.2140870336484175
.9098673054587254	.7332875526907915	.5576965425705864
.8739411604116814	.8056690124101580	.4519200877536995
.8218340674728559	.7272263891958599	.5656503207382451
.9434542763731342	.9216676908717178	.3593239342084407
.8978786466489923	.3648662069964927	.3892532379540150
.8297009483275679	.2492430320538961	.6129244772873209
.9130863619354656	.2385895478322183	.4902933326776169
.9211359606000236	.5158242795269269	.4974511476133314
.9164936998836167	.2448197645569390	.6179356561909102
.8319481066147557	.2634115011735302	.4843970434307420
.9168202164223083	.5114113322546231	.6245065192269934
.9869459923286114	.9304506666551552	.2417915233142247
.7588072802992861	.0157453348745982	.5434822399963667
.9923759616870629	.2496150667331398	.5471380867727152
.7553102437674241	.2619029017884734	.5460577075436824
.7478807568401966	.4944151108021317	.5072637247165300
.6902780127287569	.1606446229290513	.3065950766073282
.7286423492250081	.2806197683138027	.4225583321557754
.6673185366727723	.7732506317995534	.5234046378448581
.6903217043644791	.9052907964681441	.3077739438387401
.7500093293300872	.7562137098273206	.5122015709238883
.7283724356537746	.9019991229826865	.4239348086547667
.8665435538127030	.1727342891746455	.2909155612919959
.8312262578291145	.9319608101471785	.2148583710398924
.7222688334857587	.5793222753652002	.6149488189776664
.9058201602880629	.9947589838352797	.5540952288226690
.9489360761618837	.4408299467139618	.2801772651396301
.1645298191090440	.4996248686705328	.7235027270570782
.3796864566134443	.3158741689613858	.7231434241061534
.6649046522337170	.5010810548556829	.7239389449482041

.8801897326597145	.3151169265455643	.7236900144933082
.0648668310708772	.7075779374769142	.2207563970729700
.1504419469553091	.4356157302313441	.2067643650555661
.3251621004423016	.8340344402687181	.2041969450851411
.1508993159851915	.9633291286620315	.1868076033412933
.3640015685069571	.6297609405369015	.1895010996574967
.5270573031461754	.5745437353431949	.1846459439067751
.6061330484224406	.8491465210933785	.2145167536436446
.5073448001134078	.9594936547425184	.2134860297152590
.6927223376489058	.5463525729261114	.2092731586170208
.8261694943708549	.5224839212299571	.1760250847982726
.9725710173358465	.8269735590971110	.2288286728504933
.8607048814809179	.9730055724707105	.1872012257565039
.1935332622718924	.5120336907282816	.7470561475159591
.4077212097844684	.3316969629358295	.7502281374355153
.6786359426750123	.4492377953817788	.7482719200858683
.9073157606972402	.3854386401654593	.7515293362764400

Frequency of vibration in 001-1 in cm-1

1 3834.987927
2 3829.008046
3 3827.445568
4 3826.270303
5 3421.133204
6 3413.096299
7 3376.792157
8 3375.492766
9 1127.786716
10 1124.396106
11 1119.718713
12 1113.518105
13 1109.388721
14 1089.641998
15 1084.600367
16 1071.511429
17 1065.792944
18 1060.639213
19 1054.186362
20 1033.290132
21 1028.368691
22 986.556124
23 984.598827
24 976.446852
25 972.346654
26 969.299373
27 967.459638
28 960.052364
29 959.912294
30 958.496869
31 927.833179

32 925.278978
33 875.012201
34 868.706704
35 847.234539
36 847.123511
37 806.345411
38 802.786477
39 769.548837
40 768.853010
41 736.708796
42 731.963531
43 721.103403
44 717.394101
45 713.304311
46 705.261669
47 704.463013
48 703.092069
49 700.816178
50 668.760045
51 668.440063
52 646.189771
53 608.261556
54 598.213767
55 579.528109
56 568.303614
57 558.262331
58 553.295825
59 527.965346
60 500.409884
61 485.293610
62 463.739749
63 462.490061
64 452.551044
65 445.329666
66 429.470117
67 426.566018
68 423.875761
69 413.440827
70 408.665620
71 406.250536
72 404.478016
73 389.771240
74 386.343654
75 379.998884
76 372.122063
77 370.359948
78 366.973311
79 365.315634
80 359.935680
81 355.060658
82 350.294440

83 346.393226
84 338.579259
85 331.890251
86 327.698546
87 318.900426
88 314.090700
89 306.787521
90 302.344379
91 299.659447
92 286.755410
93 280.557669
94 277.049353
95 272.386868
96 262.270014
97 254.933060
98 247.223859
99 235.213932
100 223.659453
101 217.904702
102 215.838823
103 208.606477
104 204.077965
105 197.010643
106 192.756487
107 187.759112
108 178.788088
109 176.664415
110 171.343249
111 165.540307
112 159.690907
113 153.360549
114 146.349897
115 136.941765
116 136.188415
117 128.378962
118 119.185455
119 114.223406
120 89.670676

frequency of vibration in 001-2 in cm-1

1 3875.230924
2 3870.348698
3 3827.271170
4 3824.714184
5 3410.920455
6 3378.364698
7 1142.638115
8 1134.802948
9 1127.762120
10 1124.081640

11 1113.847537
12 1099.602702
13 1094.558289
14 1085.528796
15 1082.206604
16 1067.596696
17 1041.566930
18 1001.816948
19 987.487300
20 984.114000
21 973.596856
22 971.060886
23 970.410246
24 967.094645
25 962.110547
26 958.912292
27 906.491084
28 904.278604
29 889.112471
30 869.082252
31 845.020485
32 802.768197
33 795.935413
34 770.334378
35 762.849221
36 724.656716
37 717.169053
38 716.366854
39 710.802202
40 709.394267
41 706.656893
42 694.515025
43 690.967552
44 679.679054
45 669.657734
46 634.554784
47 610.925905
48 594.445270
49 566.262419
50 561.930517
51 556.667160
52 549.856080
53 528.209165
54 499.983312
55 485.926743
56 461.398111
57 450.084865
58 444.930369
59 438.694468
60 425.707957
61 416.530081

62 407.701747
63 402.449889
64 399.470296
65 398.784370
66 389.955717
67 388.764354
68 376.650155
69 372.679744
70 370.601254
71 361.067516
72 359.519181
73 358.487677
74 352.639303
75 347.351775
76 339.848382
77 335.457148
78 330.454865
79 322.226686
80 311.148664
81 304.533766
82 303.818470
83 299.292340
84 290.406438
85 288.502772
86 280.364385
87 270.712558
88 264.306287
89 255.763115
90 249.690404
91 242.570184
92 232.218719
93 214.447800
94 207.193816
95 202.554088
96 198.509761
97 187.826402
98 180.544231
99 169.072461
100 160.872038
101 155.901750
102 148.629157
103 142.705640
104 136.811774
105 129.793049
106 122.213298
107 111.577707
108 107.886554
109 85.970978
110 81.633144
111 72.504671

frequency of vibration in H2O in cm-1

1 3856.459785
2 3738.825865
3 1578.166553
