

Under what conditions does (SiO)_N nucleation occur? A bottom-up kinetic modelling evaluation

Stefan T. Bromley^{*1,2}

¹*Departament de Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, C/ Martí i Franquès 1, E-08028 Barcelona, Spain*

²*Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain*

Juan Carlos Gomez Martin³, John M. C. Plane^{*3}

³*School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK*

* Corresponding authors: s.bromley@ub.edu, J.M.C.Plane@leeds.ac.uk

Supplementary Information 1

Optimised atomic coordinates of (SiO)_N (N = 1 – 20) cluster isomers employed:

SiO					
1	Si	-0.007668	0.000000	0.000000	
2	O	1.507668	0.000000	0.000000	
(SiO) ₂					
1	O	1.641245	-1.802696	-0.815961	
2	Si	2.333893	-0.590239	0.164347	
3	Si	0.476751	-2.216124	0.360423	
4	O	1.169440	-1.003709	1.340755	
(SiO) ₃					
1	Si	2.723070	-3.031762	-1.481620	
2	O	1.201146	-3.246976	-0.806589	
3	Si	2.648030	-0.494064	0.349631	
4	Si	0.208573	-2.454856	0.291403	
5	O	1.138354	-1.125721	0.723988	
6	O	3.240177	-1.607946	-0.758013	
(SiO) ₄					
1	O	-0.323417	-3.331445	-0.564446	
2	Si	0.086085	-3.522938	-2.173348	
3	Si	3.340710	-2.973769	-1.851383	
4	O	1.744627	-3.347731	-2.158558	
5	Si	2.302349	-0.483837	-0.110394	

6	Si	0.089054	-2.720995	0.935606
7	O	1.164401	-1.503066	0.558831
8	O	3.232591	-1.519480	-1.035078

(SiO)₅

1	Si	3.073825	1.214661	-1.816759
2	O	2.259288	0.060106	-0.849615
3	Si	2.257843	2.570898	0.670284
4	Si	3.623380	4.432778	2.698362
5	Si	1.557748	0.198515	0.668989
6	O	2.265213	5.348560	2.328305
7	O	1.079381	3.742642	0.639708
8	O	3.399514	3.058455	1.775496
9	O	2.992019	2.553293	-0.840302
10	Si	0.895780	5.237358	1.362623

(SiO)₆

1	O	2.795470	0.741278	0.650827
2	Si	3.166859	-0.867139	0.844741
3	Si	1.070959	-1.707009	-1.512121
4	O	2.322470	-1.591492	-0.417323
5	Si	-0.338189	0.044565	-0.481031
6	Si	1.934007	2.103543	0.179292
7	Si	-2.268178	-0.492884	1.856822
8	O	-3.360855	-0.019023	0.675592
9	O	0.481255	1.485464	-0.327671
10	O	-0.802850	-0.414251	1.057189
11	O	-1.729214	0.383620	-1.324742
12	Si	-3.348346	0.465776	-0.934909

(SiO)₇

1	Si	2.943979	-1.609101	-0.910794
2	Si	-0.002272	3.354301	-0.864786
3	O	-1.304156	2.325479	-0.567533
4	O	1.316255	2.356773	-0.535910
5	Si	1.334631	0.783861	-0.038517
6	O	-1.295605	-2.295782	-0.642926
7	O	2.702459	0.021473	-0.557757
8	Si	0.005618	-0.022449	1.824545
9	O	1.419761	-2.263434	-0.610145
10	Si	0.046461	-1.510701	-0.091275
11	Si	-1.296993	0.752463	-0.070205
12	O	0.040246	0.025326	-1.096135
13	O	-2.633368	-0.042189	-0.621937
14	Si	-2.827302	-1.677922	-0.980402

(SiO)₈

1	Si	1.178896	-0.042242	2.318213
2	Si	-1.332133	2.949868	-0.952381
3	O	2.335132	1.329905	-0.596934
4	Si	-1.617657	0.012996	-0.510911
5	Si	0.977806	1.301517	0.359307
6	Si	0.972735	-1.315273	0.313109
7	Si	-1.314612	-0.042005	2.594722

8	Si	3.221571	0.015459	-1.177986
9	O	0.004281	-2.593218	-0.102084
10	O	0.072864	0.011029	-0.583111
11	O	-2.038483	-1.373643	-1.247717
12	O	2.329988	-1.315228	-0.643687
13	O	-2.033148	1.426332	-1.198367
14	O	-2.046588	-0.013772	1.054895
15	O	0.014242	2.596937	-0.010633
16	Si	-1.343412	-2.907591	-1.055524

(SiO)₉

1	Si	-1.112952	-2.090169	2.339722
2	Si	-0.381666	-0.789018	4.058092
3	Si	1.976340	3.245960	-0.896582
4	O	2.538421	-1.044600	-0.954703
5	Si	-0.544851	1.691120	-0.299025
6	Si	1.898789	0.289419	-0.277632
7	Si	-0.819108	-1.610712	0.147072
8	Si	0.130422	0.072686	2.010527
9	Si	1.853078	-2.532187	-1.343591
10	O	-2.067013	-1.080427	-0.782922
11	O	0.358375	0.425572	-0.894218
12	O	1.682990	0.119484	1.332113
13	O	-2.010047	1.565121	-0.995066
14	O	0.280432	-2.427238	-0.762694
15	O	0.316240	3.033630	-0.665207
16	O	-0.604486	1.430951	1.312051
17	O	2.627993	1.707478	-0.645498
18	Si	-2.943185	0.219666	-1.386069

(SiO)₁₀

1	Si	-4.626480	0.833484	-2.085093
2	Si	-3.249987	-0.603406	-0.984490
3	Si	-2.776592	1.721448	-1.102584
4	O	-1.043659	0.267993	1.186858
5	Si	1.174204	3.389051	1.637331
6	O	-0.360987	2.845777	1.204048
7	Si	1.923982	1.039011	-0.092070
8	Si	-1.397907	-1.127670	0.364360
9	Si	-0.840697	1.603943	0.225416
10	Si	1.360579	-1.722228	0.049063
11	Si	-0.214433	-3.411433	1.983649
12	O	2.480484	-1.934642	-1.126219
13	O	0.458309	1.355825	-0.770800
14	O	1.798648	-0.331124	0.808267
15	O	-0.125384	-1.505691	-0.625059
16	O	1.168240	-2.920712	1.144201
17	O	3.013767	0.680505	-1.260171
18	O	-1.423495	-2.356660	1.468289
19	O	2.237903	2.318060	0.876487
20	Si	3.464038	-0.810158	-1.913869

(SiO)₁₁

1	Si	-1.608994	3.100426	-2.016203
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2	Si	6.515651	-0.004364	1.096066
3	Si	5.025724	-0.031596	-0.624612
4	Si	4.370878	0.017668	1.858776
5	O	-0.763412	-1.532059	0.748950
6	O	-3.272577	1.377803	1.673547
7	O	-2.664225	-2.638869	-0.668230
8	Si	-1.631059	-3.165789	-1.899305
9	O	-3.282549	-1.295023	1.723082
10	O	-0.251611	-2.209922	-1.711356
11	Si	-2.363374	-1.419989	0.379449
12	Si	-2.352970	1.446246	0.326153
13	O	-2.576139	-0.000759	-0.436246
14	Si	2.819316	-0.009606	0.122355
15	O	1.850284	1.321627	-0.160901
16	Si	0.256946	1.152509	-0.566874
17	Si	0.248628	-1.178504	-0.523098
18	Si	-3.876785	0.059261	2.542272
19	O	1.840696	-1.343586	-0.110528
20	O	-0.752133	1.560600	0.691119
21	O	-2.645463	2.627412	-0.766155
22	O	-0.236428	2.142255	-1.792840

(SiO)₁₂

1	Si	5.302130	0.937441	0.784435
2	Si	3.158221	0.737379	0.126071
3	Si	4.803170	-0.891447	-0.799044
4	Si	2.837412	-1.548888	0.271567
5	Si	3.887758	-0.579817	2.117355
6	Si	-3.683723	0.557383	2.727700
7	O	-3.011018	1.747957	1.740076
8	Si	-2.239715	1.651104	0.302836
9	O	-2.716681	0.229387	-0.374207
10	Si	-2.595925	-1.164230	0.490481
11	O	-3.345621	-0.881966	1.914058
12	O	-3.165258	-2.397120	-0.416791
13	Si	-2.372536	-3.250753	-1.637604
14	O	-0.810328	-2.628454	-1.593758
15	Si	-0.000550	-1.660295	-0.549237
16	O	-0.997187	-1.461708	0.739024
17	O	1.414224	-2.329594	-0.083662
18	O	1.918583	1.733827	-0.367400
19	Si	0.382043	1.357602	-0.753053
20	O	0.319839	-0.207902	-1.232898
21	O	-0.613459	1.575848	0.534417
22	O	-2.508108	2.856930	-0.764769
23	Si	-1.554150	3.318252	-2.078815
24	O	-0.194428	2.341433	-1.930742

(SiO)₁₃

1	Si	3.765827	-2.165091	2.192978
2	O	3.715840	-0.510425	2.399060
3	Si	-5.341950	-1.412914	1.285342
4	Si	-3.356675	-0.970307	0.319589
5	Si	-5.242754	0.588943	-0.158222

6	Si	-3.176085	1.311474	0.647753
7	Si	-3.835435	0.093465	2.526482
8	Si	3.994908	1.113463	2.656748
9	O	2.886690	-2.385050	0.793115
10	Si	2.072464	-1.554294	-0.342867
11	O	2.637528	-0.028315	-0.466858
12	Si	2.271606	1.459358	0.092806
13	O	3.170686	1.829654	1.395632
14	O	2.517900	2.547387	-1.109094
15	Si	1.503296	3.435826	-2.102135
16	O	-0.019866	2.854269	-1.694091
17	Si	-0.528649	1.745820	-0.606523
18	O	0.677802	1.529431	0.479315
19	O	-1.889211	2.235559	0.152383
20	O	-2.148062	-1.803021	-0.463609
21	Si	-0.727215	-1.270993	-1.055077
22	O	-0.830947	0.331918	-1.370486
23	O	0.474606	-1.525687	0.029303
24	O	2.211338	-2.282756	-1.804845
25	Si	1.117249	-2.701806	-3.002304
26	O	-0.325877	-2.063998	-2.427389

(SiO)₁₄

1	O	4.033408	0.032602	-0.358279
2	O	1.493871	2.671423	-1.647355
3	O	4.417071	1.402825	1.822273
4	Si	4.939626	0.084710	2.741915
5	O	3.960970	2.707520	-0.619024
6	O	4.446626	-1.269122	1.858554
7	Si	3.646364	1.450487	0.380558
8	Si	1.045340	1.411243	-0.709434
9	O	2.017985	1.491093	0.611802
10	Si	3.040066	-3.497839	-1.629652
11	O	1.552221	-2.695555	-1.573679
12	Si	1.076270	-1.420165	-0.670464
13	Si	-1.429848	-0.022864	-0.050709
14	Si	3.677346	-1.372792	0.419025
15	Si	2.963821	3.504289	-1.725353
16	O	4.019452	-2.649425	-0.546089
17	O	2.050195	-1.442543	0.652046
18	O	1.329831	-0.012449	-1.483667
19	O	-0.519363	1.331884	-0.252785
20	O	-0.489793	-1.362417	-0.215312
21	O	-2.625468	-0.051822	-1.182641
22	Si	-7.270314	-0.077385	0.876631
23	Si	-6.416207	-0.099471	-1.424639
24	Si	-5.379907	1.315179	0.733951
25	Si	-4.225469	-0.064956	-0.783436
26	Si	-5.347894	-1.428922	0.772115
27	O	-2.147921	-0.010403	1.408332
28	Si	-3.704915	-0.019339	2.064149

(SiO)₁₅

1	Si	-5.414472	-1.567466	-1.830260
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2	Si	-3.563003	-0.902068	0.854529
3	Si	-3.525916	-0.257492	-1.335823
4	Si	-3.316601	-2.683762	-0.856415
5	Si	-5.568791	0.257108	-0.028204
6	O	-2.467942	-0.396885	1.997509
7	Si	-1.185023	0.583529	1.739601
8	O	-1.480900	1.483144	0.401438
9	Si	-1.135714	1.449425	-1.200812
10	O	-2.401151	0.776980	-1.988189
11	O	-0.816040	2.955829	-1.758303
12	Si	0.562761	3.713960	-2.354213
13	O	1.795756	2.624950	-1.975626
14	Si	1.692828	1.250203	-1.103141
15	O	0.232392	0.579772	-1.449803
16	O	2.884084	0.162195	-1.313911
17	Si	3.615201	-0.781078	-0.179615
18	O	2.841146	-0.595665	1.261715
19	Si	1.646868	0.443693	1.636918
20	O	1.699127	1.629688	0.497757
21	O	0.182689	-0.294572	1.519681
22	O	-0.896597	1.544563	3.033995
23	Si	0.456185	1.846643	3.987773
24	O	1.710203	1.125549	3.117715
25	O	3.544367	-2.343105	-0.640410
26	O	5.178707	-0.338022	-0.023199
27	Si	6.636897	-1.137898	-0.233412
28	Si	4.701186	-3.512134	-0.964310
29	O	6.127921	-2.669842	-0.692142
30	Si	-5.453271	-2.254611	0.501413

(SiO)₁₆

1	Si	2.349636	-1.639299	0.040297
2	Si	5.029400	0.512744	-1.230189
3	Si	3.018148	-0.706576	2.074352
4	Si	3.232485	-0.877338	-1.982066
5	Si	4.827580	-1.620071	0.171705
6	Si	2.933128	0.805069	-0.030180
7	Si	4.891079	0.623476	1.402876
8	O	-2.077501	3.024118	-2.253093
9	Si	0.445853	2.591014	-0.256656
10	O	-0.331598	1.438006	-1.136200
11	O	-2.913139	-0.887235	2.898318
12	Si	-1.585643	1.660158	1.447145
13	O	2.007801	2.196275	-0.133537
14	Si	-3.199121	0.554152	3.744079
15	O	1.168337	-2.813711	0.033609
16	O	-1.033062	0.118854	1.423798
17	Si	-2.067548	-1.146375	1.525381
18	O	0.128039	3.988385	-1.059662
19	O	-0.281396	2.626526	1.233845
20	Si	-0.444708	-2.754390	-0.101243
21	O	-1.159084	-4.025934	-0.851944
22	O	-2.456691	1.768999	2.825283
23	Si	-1.058618	4.381592	-2.195594

24	O	-3.076629	-1.121167	0.219157
25	O	-2.974013	-2.476520	-2.099491
26	Si	-1.945696	1.654907	-1.373524
27	O	-0.821303	-1.461386	-1.043434
28	O	-2.584024	0.290564	-2.017371
29	Si	-2.420673	-1.167938	-1.292786
30	O	-2.560347	1.898375	0.137204
31	O	-1.156772	-2.499958	1.373285
32	Si	-2.418663	-4.076560	-1.981202

(SiO)₁₇

1	Si	-3.596666	0.648158	-3.448325
2	O	-2.696352	1.791347	-2.638298
3	Si	2.147651	-1.822062	-0.087442
4	Si	4.962154	0.072077	-1.456531
5	Si	2.998365	-0.994385	1.924434
6	Si	3.016720	-1.140635	-2.145040
7	Si	4.617670	-2.055173	-0.066047
8	Si	2.946662	0.528303	-0.167880
9	Si	4.949516	0.168341	1.170189
10	O	-1.621974	4.156820	-1.872433
11	Si	0.685244	2.687136	-0.288698
12	O	-0.294351	1.949215	-1.395167
13	O	-3.036868	-0.608052	2.739334
14	Si	-1.567108	1.832290	1.220397
15	O	2.130931	1.976227	-0.224260
16	Si	-3.164952	0.835000	3.603094
17	O	0.863683	-2.864261	-0.055497
18	O	-1.281312	0.242101	0.993142
19	Si	-2.306504	-0.981791	1.328754
20	O	0.766494	4.260949	-0.736486
21	O	-0.111571	2.578360	1.155435
22	Si	-0.751037	-2.883637	-0.093147
23	O	-1.371431	-4.358581	-0.434669
24	O	-2.369570	1.963872	2.635966
25	Si	-0.336047	5.206969	-1.589807
26	O	-3.413691	-1.123036	0.118935
27	O	-3.514457	-3.250795	-1.529788
28	Si	-1.820043	2.564736	-1.525460
29	O	-1.315212	-1.861230	-1.259487
30	O	-3.424531	-0.745882	-2.550651
31	Si	-2.957012	-1.716428	-1.348096
32	O	-2.479294	2.402719	-0.024398
33	O	-1.397760	-2.344284	1.328014
34	Si	-2.827962	-4.750218	-1.191159

(SiO)₁₈

1	Si	3.870785	-0.053305	1.480283
2	Si	5.426977	-1.381662	-1.562084
3	Si	4.363110	1.972364	0.425306
4	Si	4.302223	-2.093357	0.426422
5	Si	6.194785	-0.088359	0.524231
6	Si	3.485047	-0.048130	-0.917976
7	Si	5.465987	1.226191	-1.562837

8	O	3.088680	-0.041138	2.926486
9	O	-2.665016	-3.493815	0.946906
10	Si	-2.718988	-1.862157	1.069503
11	Si	0.453064	-0.005069	-1.114521
12	O	-1.399823	-1.325816	1.869686
13	Si	-1.809766	1.912822	-1.742532
14	O	0.481256	-0.004474	0.518263
15	Si	-2.677232	1.921809	1.064227
16	Si	-4.941823	0.055157	2.253233
17	Si	-0.457941	0.006089	1.851675
18	O	-4.054366	-1.291622	1.806690
19	Si	-1.857311	-1.869872	-1.738679
20	O	-4.026154	1.380064	1.798384
21	O	-1.883956	-3.500628	-1.598137
22	O	-1.371928	1.357283	1.867713
23	O	-2.588148	3.552004	0.942363
24	Si	-2.193142	4.580087	-0.332379
25	O	-1.801121	3.543626	-1.600808
26	O	-0.280209	1.343548	-1.662845
27	O	-0.315511	-1.334563	-1.660928
28	O	0.477921	-0.002700	3.171903
29	O	1.988954	-0.025640	-1.634194
30	Si	-2.295574	-4.529277	-0.329593
31	O	-2.509115	1.364951	-3.106992
32	Si	-3.013586	0.034531	-3.988329
33	O	-2.545810	-1.305980	-3.102094
34	Si	1.875881	-0.021563	4.066837
35	O	-2.664084	1.362891	-0.467303
36	O	-2.697894	-1.302914	-0.461798

(SiO)₁₉

1	Si	4.774970	1.964619	-1.108158
2	Si	4.752290	-0.070651	2.309368
3	Si	4.743084	-2.012535	-1.162117
4	Si	3.662773	-1.747681	0.971384
5	Si	3.690152	1.659403	1.017657
6	Si	3.681787	-0.004211	-1.955268
7	O	-3.791308	-1.295859	0.740484
8	Si	-3.272536	1.444082	-0.794290
9	O	0.501407	-1.318549	-2.290513
10	Si	-2.707969	4.051711	-2.253038
11	O	-1.138566	-0.048564	4.111401
12	Si	1.315544	-1.575385	0.881949
13	O	-1.667773	-0.009228	1.586648
14	O	0.515168	1.263578	2.328325
15	Si	-0.456278	-2.254267	-1.340382
16	O	0.527992	2.639904	0.017716
17	Si	-0.419605	2.295068	-1.277912
18	O	-1.099503	3.593278	-2.001449
19	O	-3.769994	1.333832	0.776071
20	Si	5.416127	-0.044828	0.014357
21	O	-1.156777	-3.520924	-2.099316
22	O	0.485922	-2.649758	-0.055347
23	Si	-2.772322	-3.946656	-2.362682

24	O	-3.703740	-2.726540	-1.641338
25	Si	-3.295265	-1.371600	-0.832342
26	O	-3.778598	0.049781	-1.519173
27	O	-3.688938	-0.015034	3.205366
28	Si	-0.444134	-0.033743	2.632059
29	O	0.523698	1.370898	-2.253424
30	O	0.994212	-0.009214	0.007146
31	Si	-3.287043	0.003253	1.625702
32	O	0.493911	-1.337681	2.292414
33	Si	1.340489	1.527018	0.924581
34	O	-1.653758	1.393834	-0.772802
35	Si	1.333282	0.012640	-1.783358
36	O	-1.675902	-1.348093	-0.809524
37	Si	-2.751983	-0.042307	4.618767
38	O	-3.659006	2.827013	-1.565855

(SiO)₂₀

1	O	-3.550554	4.223042	-0.087663
2	Si	-5.074357	3.551910	-0.082006
3	Si	4.499159	2.832761	-0.032362
4	Si	5.052879	-0.528341	2.019637
5	Si	5.069062	-0.599048	-1.958855
6	Si	4.163499	-1.584325	0.044908
7	Si	3.630096	1.387990	1.675638
8	Si	3.643769	1.327859	-1.694718
9	O	-3.131854	-2.364858	0.029528
10	Si	-3.552019	0.832915	-0.029541
11	O	0.847389	-0.321412	-2.667649
12	Si	-2.143077	5.120098	-0.099181
13	O	-0.561226	-2.449962	3.584794
14	Si	1.813641	-1.866687	0.040764
15	O	-1.259009	-1.150184	1.434314
16	O	0.825405	-0.225188	2.684001
17	Si	0.038731	-1.686202	-2.258913
18	O	0.196180	1.959197	1.275110
19	Si	-0.695550	2.350212	-0.045308
20	O	-0.951866	3.954644	-0.074986
21	O	-3.655867	-0.125573	1.308090
22	Si	5.522888	0.672829	0.010320
23	O	-0.532486	-2.577078	-3.499283
24	O	1.066137	-2.510513	-1.281743
25	Si	-2.079852	-3.100468	-3.928758
26	O	-3.091148	-2.502457	-2.715049
27	Si	-2.825143	-1.589889	-1.390922
28	O	-3.645453	-0.172995	-1.332689
29	O	-3.113343	-2.403968	2.777509
30	Si	0.020205	-1.604046	2.317985
31	O	0.207099	1.912291	-1.343396
32	O	1.193512	-0.161978	0.007464
33	Si	-2.836424	-1.539443	1.423710
34	O	1.055703	-2.462634	1.379649
35	Si	1.352804	0.824129	1.526497
36	O	-2.109248	1.571015	-0.037228
37	Si	1.365458	0.768947	-1.544385

38	O	-1.247667	-1.200944	-1.402773
39	Si	-2.112063	-2.958118	4.019994
40	O	-4.760859	1.910383	-0.053458