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Modelling the Atomic Arrangement of Amorphous 2D Silica: A Network Analysis

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1 Units

In order to estimate the absolute energy scale of our 2D model it is not possible to resort to experimental observables. However, a comparison may be performed with the previous quantum-mechanical DFT energies for amorphous 2D-silica. The details of the DFT analysis can be found in Ref. 1. A 360 particle system with four different ring-size distributions was optimised at constant volume. This corresponds to 150 particles on the surface. The average energy of these structures was approx. -2840 eV. In contrast, as can be seen from Fig.4 (main paper) the average energy for our 2D-silica model with 80 particles is approx. -27. Thus, the energy scale is approx. (2840/150)/(27/80) eV $\approx$ 56 eV.

As a consequence our simulation temperature of 0.015 corresponds to approx. 9700 K. Note that the binding energy of the bridging oxygen is basically constant when comparing the different disordered states. Strictly speaking one should take into account that for this reason the binding contribution of that oxygen should not be taken into account when comparing the total energy with that of the 2D system. Thus, the 9700 K should be considered as an upper bound.

We select the mass unit as the total mass of the '(top-layer silicon)-(bridging oxygen)-(bottom-layer silicon)' unit. Following this, we selected our unit of time as (using that the reduced silicon mass in the 2D model is equal to 1).

$$t_{unit} = r_{unit}\sqrt{M_{unit}/E_{unit}}.$$

Using

- Unit of length (r_{unit}) : 1.0 Å
- Unit of energy (E_{unit}) : 56 eV
- Unit of mass (M_{unit}) : 72 g/mol

This yields as a unit of time approx. 11 fs.

2 Finite size effect

We have simulated a 200 particle system at $T^* = 0.015$ to see if any finite size effect is present. We samples about ~ 1400 defect free structures from about $7 \cdot 10^4$ overall structures with about 2 % probability. This shows how fast the probability of sampling defect free structures decreases with system size. We compared $P_{eff}^{triplet}$ for the 200 and 80 particle system. As shown in Fig. 1, the results for 200 particles and 500 particles, respectively, for the effective triplet probabilities compare extremely well with our results for the 80 particle system. Since we have just a single configuration for the 500 particle system, the correlation is slightly reduced due to statistical noise. As explained in the paper (section VII.i.), $P_{eff}^{triplet}$ represent the inherent stability of the triplets, irrespective of the ring distribution. Therefore we can assert that finite size effect is not present in our model system except for probability of finding defect-free states.

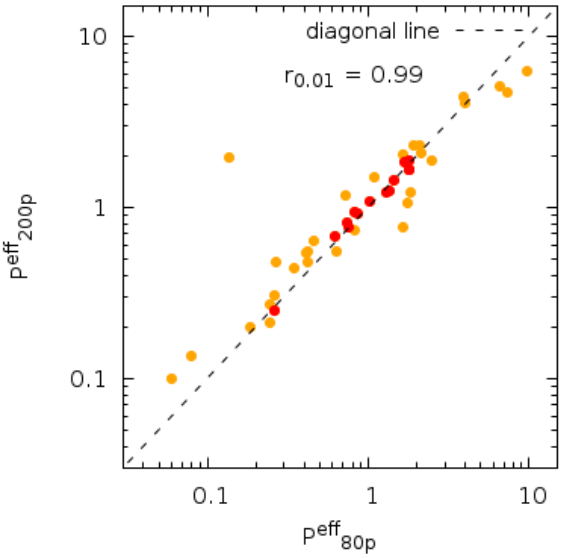

Fig. 1 The comparison of effective triplet probabilities for 80 particle and 200 particle systems. All triplets which have $P_{ijk}^{predicted} > 0.01$ as well as $P_{ijk} > 0.01$ for both 80 particle and 200 particle are marked in red. The correlation coefficient is calculated for the red points only.

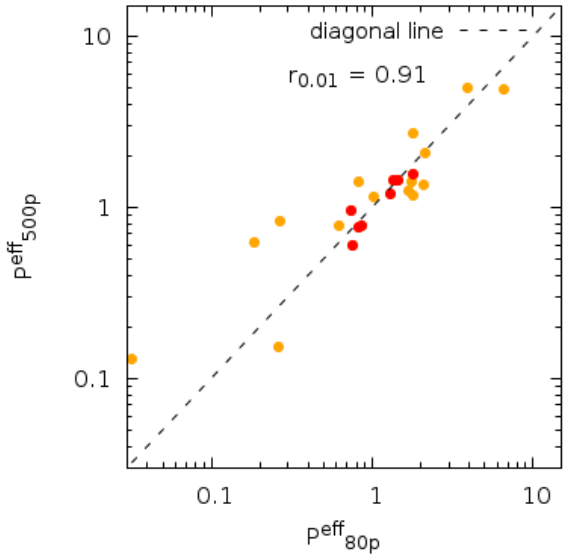

Fig. 2 The comparison of effective triplet probabilities for 80 particle and 500 particle systems. All triplets which have $P_{ijk}^{predicted} > 0.01$ as well as $P_{ijk} > 0.01$ for both 80 particle and 500 particle are marked in red. The correlation coefficient is calculated for the red points only.

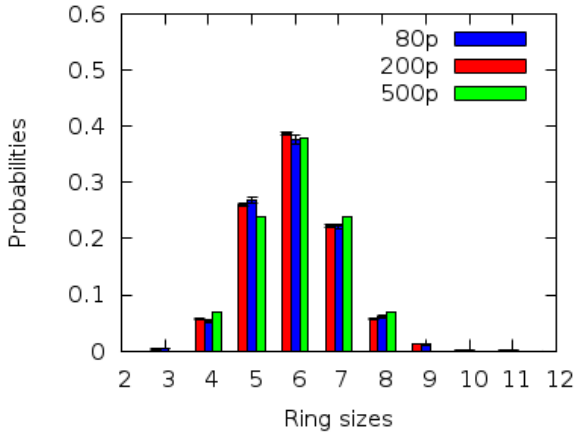

Fig. 3 The comparison of ring probabilities for 200 particle and 500 particle systems with 80 particle systems, at $T^* = 0.015$.

3 Different sets of experimental data / Unconvoluted numerical data

We have compared two different methods of generating 2D-silica coordinates as discussed in the main part in section II. Except for the first peak of the pair correlation function, the rest of the comparison in Fig. 4 and Fig. 5 gives very similar results. The data are compared with the unconvoluted numerical data.

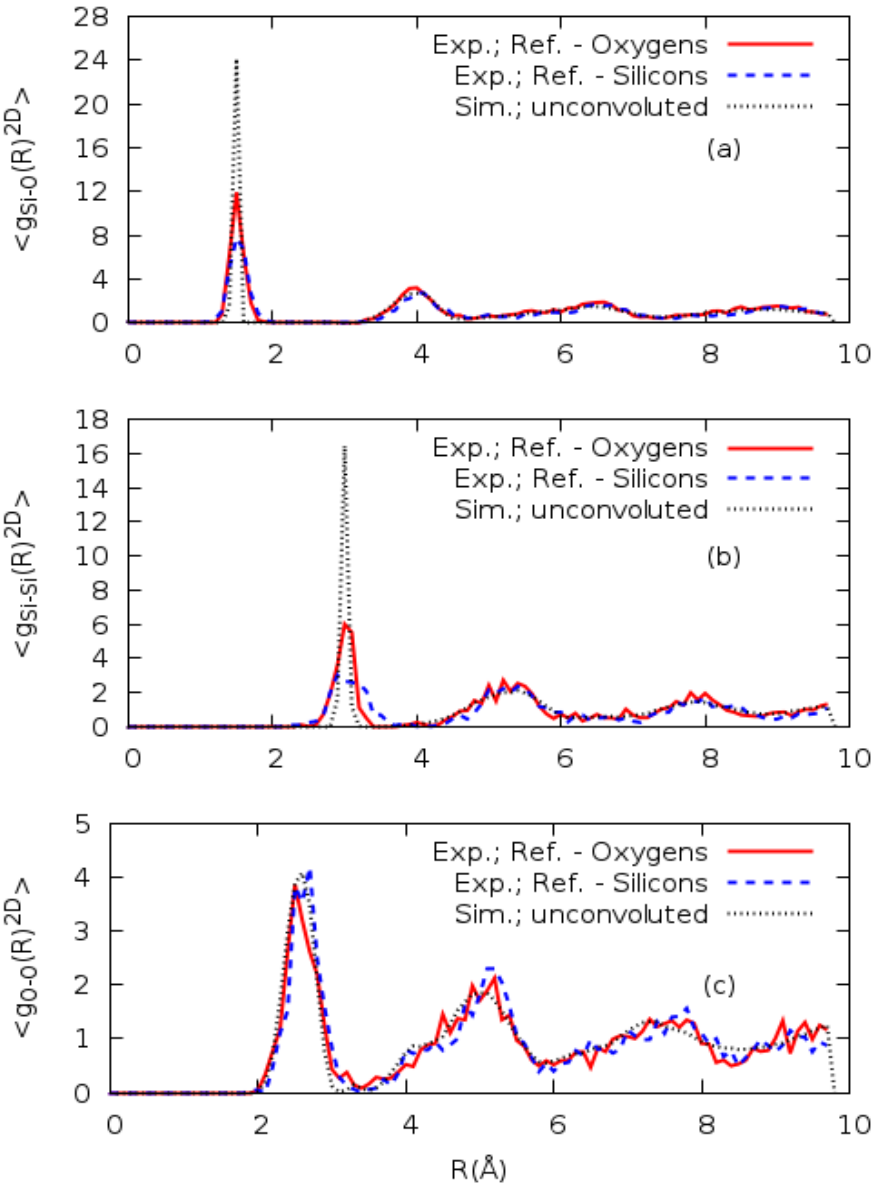

Fig. 4 Comparison of two different methods of generating 2D-silica coordinates as expressed by the two-dimensional pair correlation functions for (a)Si-O ,(b) Si-Si, and (c)O -O pairs. Reference structures are taken from Ref. 2. The broken line correspond to the numerically determined structures.

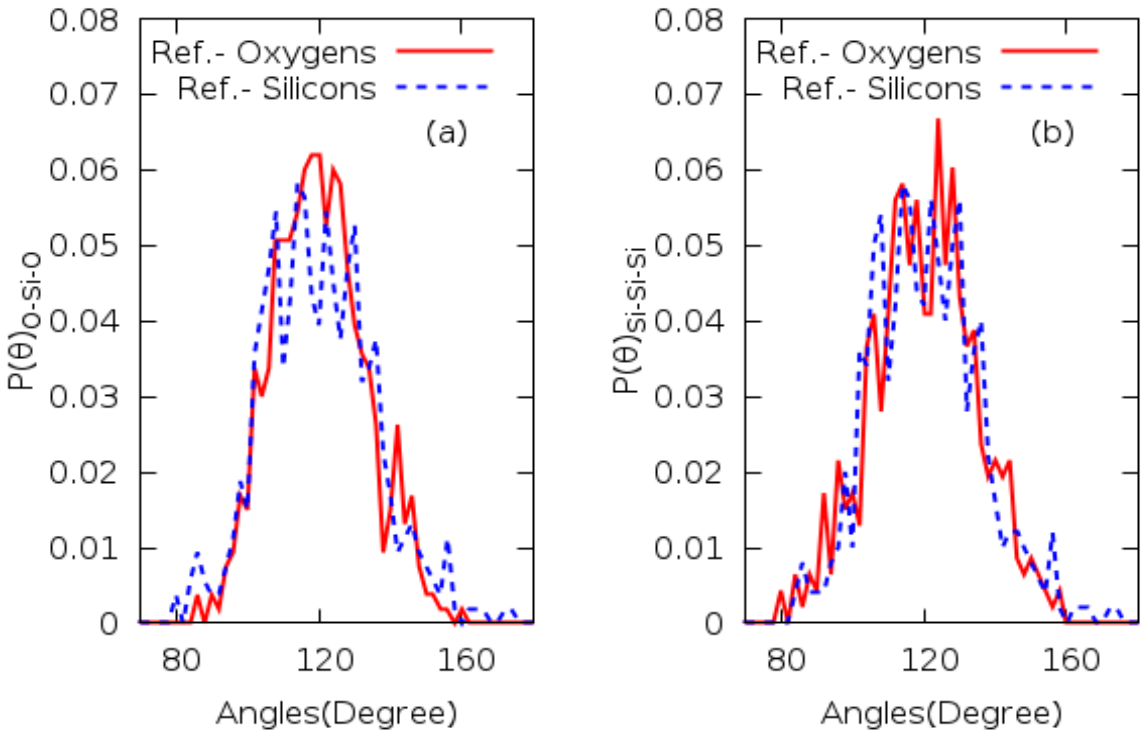

Fig. 5 Comparison of two different methods of generating 2D-silica coordinates as expressed by 2D angle distributions for (a)O-Si-O and (b) Si-Si-Si. Reference structures are taken from Ref. 2

4 Statistical errors in ring distribution

- 2D-silica, experimental data collected from Ref. 3

i	P_r	SE_r
(SE = standard error of the mean;total sample size = 317 rings,total_samples = 9)		
4	0.0379	0.0096
5	0.2744	0.0224
6	0.4448	0.0322
7	0.1609	0.0225
8	0.0757	0.0148
9	0.0063	0.0043

- Simulation data, $T^* = 0.015$

i	P_r	SE_r
(SE = standard error of the mean;each sample size = 2500 rings ,total_samples = 34)		
3	0.00382221	0.000426372
4	0.0536853	0.00295091
5	0.268602	0.00464023
6	0.377324	0.00764334
7	0.222373	0.00383898
8	0.0601644	0.00319318
9	0.0118024	0.00107203
10	0.00183472	0.000319476
11	0.000374726	8.50872e-05
12	1.00888e-05	8.90117e-06
13	1.44125e-06	1.47059e-06
14	5.76502e-06	5.88235e-06

Experimental ring probabilities corresponding to 2D-silica, experimental data collected from Ref. 3. The errorbars for the model system were calculated by dividing the frames into M=34 continuous sets, each with N=2500 subsets. For each set, the ring probabilities (P_r^m) for each rings were calculated. The standard error of the mean for each rings were calculated as,

$$SE_r = \sqrt{\frac{1}{M(M-1)}\sum_m (P_r^m - P_r)^2} \tag{1}$$

For the experimental structure, we divided the datasets into 9 blocks with equal area. As shown in Fig. 9(main paper) only rings with no open edge were taken into account. The ring-size distribution for each set were calculated and errorbars were determined from Eqn. 1.

Table 1 Ring statistics in each block of Fig. 10(main paper)

Block	Ring-size 4	Ring-size 5	Ring-size 6	Ring-size 7	Ring-size 8	Ring-size 9
I	1	10	12	1	4	1
II	1	7	18	4	2	0
III	0	10	13	4	2	0
IV	4	12	12	9	6	0
V	2	9	31	13	1	0
VI	1	14	18	5	5	1
VII	1	8	7	5	1	0
VIII	2	9	17	4	2	0
IX	0	8	13	6	1	0
Total count	12	87	141	51	24	2

5 Ring neighborhood

Experimental duplet and triplet probabilities corresponding to 2D-silica, experimental data collected from Ref. 3. Original datasets were filtered for ring sizes between 4 and 9. Errorbars were calculated similarly as rings using Eqn. 1. Triplets and duplets were assigned to the respective boxes in which the corners and major part of the edges reside.

5.1 Duplets

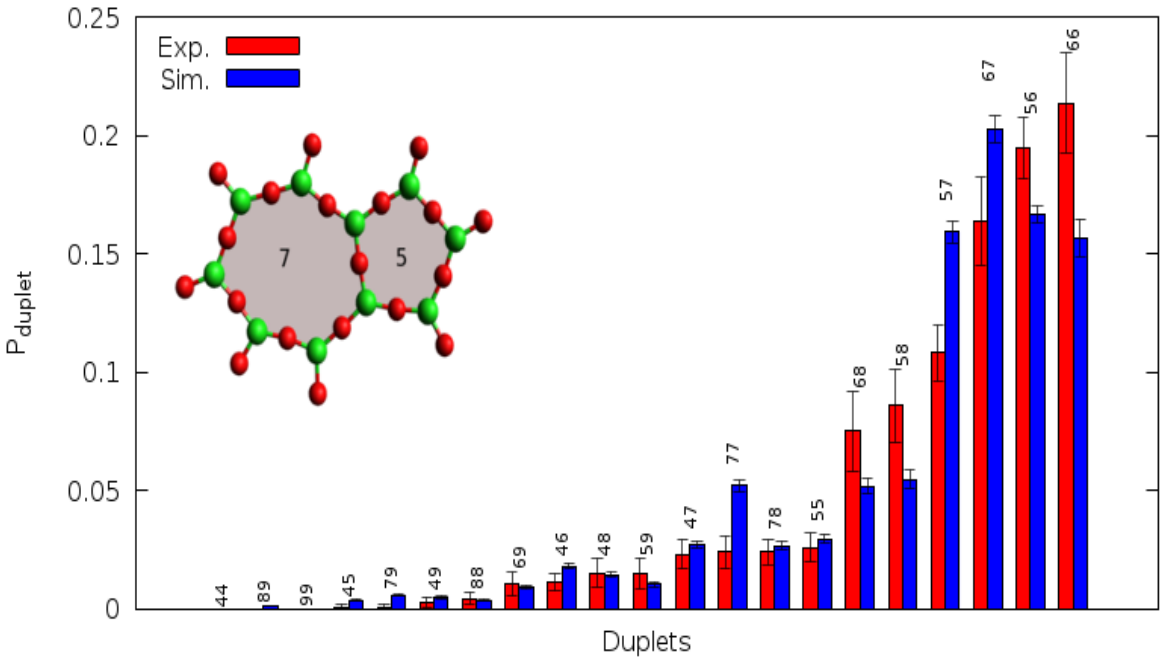

Fig. 6 Comparison of duplet distribution. The inset shows how a 'duplet' of rings was selected from a network (green = Si, red = Ox). Experimental data were calculated from Ref. 3

- 2D-silica, experimental data collected from Ref. 3

ij	P_{duplet}	SE_{duplet}

(SE = standard error of the mean;total sample size = 1119 duplets,total_samples = 9)
44 0 0
45 0.00089366 0.00091075
46 0.011618 0.0036037
47 0.023235 0.0061744
48 0.015192 0.0061735
49 0.002681 0.0019555
55 0.025916 0.0060247
56 0.19482 0.013068
57 0.10813 0.01199
58 0.085791 0.015689
59 0.015192 0.0065635
66 0.21358 0.021048
67 0.16354 0.018615
68 0.075067 0.017095
69 0.010724 0.0051336

77 0.024129 0.0069892
78 0.024129 0.0051909
79 0.00089366 0.0010101
88 0.0044683 0.0023503
89 0 0
99 0 0

- Simulation data, $T^* = 0.015$

ij	P_{duplet}	SE_{duplet}

(SE = standard error of the mean; each sample size = 2500 duplets,total_samples = 31)
44 6.04658e-05 2.78172e-05
45 0.00363785 0.000393017
46 0.0181702 0.00122897
47 0.0270879 0.00163713
48 0.0145102 0.00111864
49 0.00503378 0.000514818
55 0.0296358 0.00158064
56 0.166708 0.00345713
57 0.159138 0.00467863
58 0.0548594 0.00378236
59 0.0105763 0.00115299
66 0.156669 0.00797451
67 0.202879 0.00572938
68 0.0517353 0.00317807
69 0.00902791 0.000886107
77 0.052349 0.00253977
78 0.026777 0.00174385
79 0.00600175 0.000699169
88 0.00358599 0.000409112
89 0.00146916 0.000168614
99 8.8353e-05 2.3941e-05

5.2 Triplets

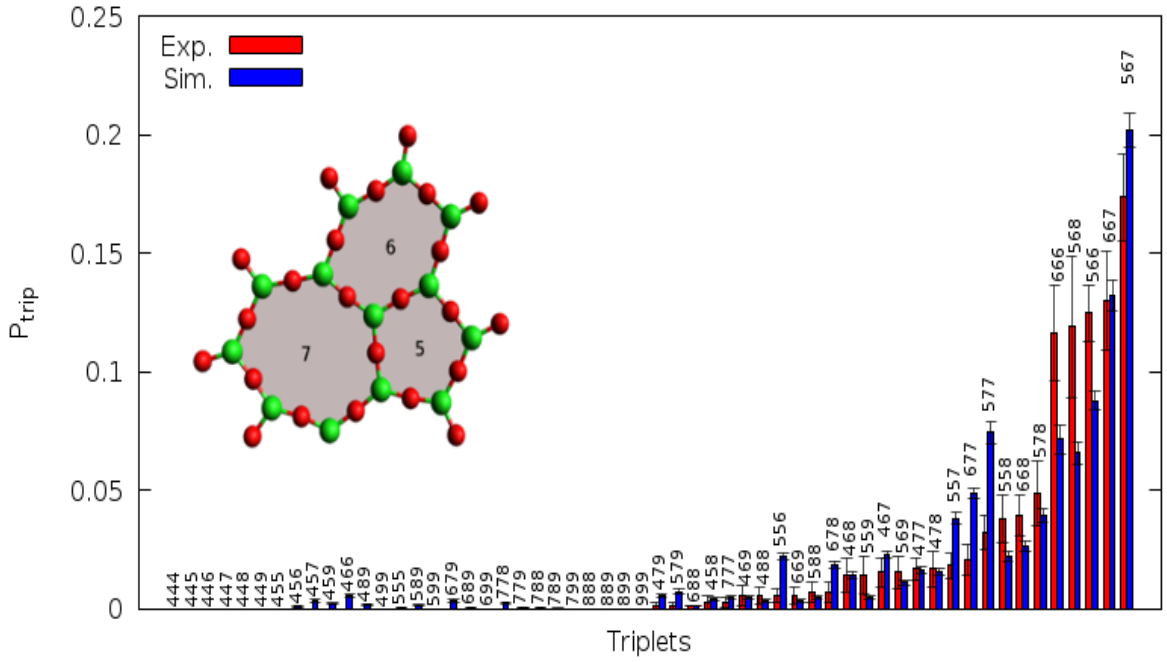

Fig. 7 Comparison of the triplet distribution. The inset shows how a 'triplet' of rings is selected from a network(green = Si, red = Ox). Experimental data were calculated from Ref. 3

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- 2D-silica, experimental data collected from Ref. 3

ijk	$P_{triplet}$	$SE_{triplet}$

(SE = standard error of the mean;total sample size = 714 triplets,total_samples = 9)

444 0 0
445 0 0
446 0 0
447 0 0
448 0 0
449 0 0
455 0 0
456 0 0
457 0 0
458 0.0028011 0.002849
459 0 0
466 0 0
467 0.015406 0.0062561
468 0.014006 0.0072313
469 0.0056022 0.0039917
477 0.016807 0.004439
478 0.016807 0.0078241
479 0.0014006 0.0014245
488 0.0056022 0.0035458
489 0 0

```
499 0 0
555 0 0
556 0.0056022 0.0026979
557 0.018207 0.0056298
558 0.037815 0.010201
559 0.014006 0.0078993
566 0.12465 0.012168
567 0.17367 0.018188
568 0.11905 0.029948
569 0.015406 0.0067741
577 0.032213 0.007326
578 0.04902 0.01366
579 0.0014006 0.0016584
588 0.0070028 0.0044268
589 0 0
599 0 0
666 0.11625 0.020083
667 0.13025 0.020802
668 0.039216 0.0085847
669 0.0056022 0.0034705
677 0.021008 0.0063797
678 0.0070028 0.0044132
679 0 0
688 0.0014006 0
689 0 0
699 0 0
777 0.0028011 0.0020738
778 0 0
779 0 0
788 0 0
789 0 0
799 0 0
888 0 0
889 0 0
899 0 0
999 0 0
```

- Simulation data, $T^* = 0.015$

ijk	$P_{triplet}$	$SE_{triplet}$

```
( SE =  standard error of the mean; each sample size = 2500 triplets,total_samples = 31)
444  0  0
445  0  0
446  2.34566e-06  1.77907e-06
447  6.09871e-05  1.35542e-05
448  7.89704e-05  6.69137e-05
449  3.90943e-05  2.10981e-05
455  2.85388e-05  1.44285e-05
```

```
456  0.00101919  0.000184709
457  0.0035482  0.000567677
458  0.00403336  0.000549385
459  0.00225574  0.000302255
466  0.00552871  0.000761401
467  0.0228799  0.00158675
468  0.0144774  0.00135721
469  0.00507209  0.000560617
477  0.0166217  0.00154753
478  0.0159282  0.00142646
479  0.005542  0.000828545
488  0.00352591  0.000487241
489  0.001882  0.000248347
499  0.000135657  4.58456e-05
555  0.000638409  0.000155202
556  0.022202  0.00133446
557  0.0382748  0.00250689
558  0.0218994  0.0021411
559  0.00458732  0.000730238
566  0.0879257  0.0040103
567  0.202056  0.00727585
568  0.0657042  0.00453187
569  0.0110891  0.00131459
577  0.0743022  0.00447254
578  0.0393542  0.00298276
579  0.00730085  0.000997223
588  0.00499351  0.000769049
589  0.0017006  0.000242169
599  0.000103991  4.32923e-05
666  0.0715319  0.00602833
667  0.132147  0.00656447
668  0.0264434  0.00210282
669  0.00336523  0.000522061
677  0.0485355  0.00206534
678  0.0187809  0.00144184
679  0.00355641  0.000510799
688  0.00137846  0.000193776
689  0.000599706  0.000118723
699  1.79834e-05  1.05601e-05
777  0.00482736  0.00063469
778  0.00241368  0.000328217
779  0.000691968  0.00021616
788  0.000615344  0.000184782
789  0.000209545  0.000101794
799  6.25508e-06  3.22076e-06
888  7.93614e-05  4.81577e-05
889  6.64602e-06  6.04749e-06
899  1.17283e-06  1.20968e-06
999  0  0
```

6 Sample Coordinates

The only structure we have sampled so far with 500 particles at $T^* = 0.015$ is given in the main paper (Fig. 3). Although the ring distribution is symmetrical as compared to lognormal in experimental, the structural properties like g(r) and angle distribution is same as 80 particle system.

- Experimental coordinates collected from Ref. 2, with Z = 0.0

```
477

Si    0.23148    1.55086    0.00000
Si    0.20524    2.85295    0.00000
Si    0.21665    3.93361    0.00000
Si    0.23553    0.93100    0.00000
Si    0.26030    2.12188    0.00000
Si    0.27881    4.54857    0.00000
Si    0.28056    3.36820    0.00000
Si    0.35574    2.59708    0.00000
Si    0.37520    3.07349    0.00000
Si    0.44380    0.52889    0.00000
Si    0.49409    3.56399    0.00000
Si    0.52735    0.23988    0.00000
Si    0.51041    1.01537    0.00000
Si    0.51867    3.87765    0.00000
Si    0.53896    1.54228    0.00000
Si    0.57888    4.55923    0.00000
Si    0.54253    2.08343    0.00000
Si    0.67124    1.27227    0.00000
Si    0.65658    1.82572    0.00000
Si    0.65490    0.74256    0.00000
Si    0.66826    2.57149    0.00000
Si    0.74389    4.81857    0.00000
Si    0.67379    3.07120    0.00000
Si    0.71331    3.36904    0.00000
Si    0.79043    4.33058    0.00000
Si    0.75912    2.27129    0.00000
Si    0.80444    4.01972    0.00000
Si    0.86059    2.83104    0.00000
Si    0.94289    0.67696    0.00000
Si    1.02259    0.40574    0.00000
Si    0.96282    1.36750    0.00000
Si    0.95559    1.87007    0.00000
Si    1.01948    3.38108    0.00000
Si    1.03361    2.16804    0.00000
Si    1.07751    3.91530    0.00000
Si    1.09489    4.42737    0.00000
Si    1.11322    1.61617    0.00000
Si    1.16534    3.64467    0.00000
Si    1.16701    0.85619    0.00000
Si    1.18704    1.15316    0.00000
Si    1.14315    2.84844    0.00000
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Si    1.21259    4.72203    0.00000
Si    1.29287    2.59128    0.00000
Si    1.23924    4.15199    0.00000
Si    1.30962    2.28210    0.00000
Si    1.30188    0.33316    0.00000
Si    1.40562    1.55037    0.00000
Si    1.46158    0.81536    0.00000
Si    1.44230    3.26592    0.00000
Si    1.47624    1.25975    0.00000
Si    1.47217    3.57930    0.00000
Si    1.53640    0.51703    0.00000
Si    1.54182    2.08921    0.00000
Si    1.50934    4.75361    0.00000
Si    1.60926    1.78336    0.00000
Si    1.53386    4.10805    0.00000
Si    1.59433    2.73069    0.00000
Si    1.64629    3.83252    0.00000
Si    1.65523    3.04794    0.00000
Si    1.66424    1.03809    0.00000
Si    1.74569    4.31961    0.00000
Si    1.77210    4.61774    0.00000
Si    1.79739    2.25816    0.00000
Si    1.85269    2.55088    0.00000
Si    1.83271    0.45780    0.00000
Si    1.91761    1.72669    0.00000
Si    1.95845    0.98050    0.00000
Si    1.95014    3.13991    0.00000
Si    2.01858    3.44220    0.00000
Si    1.92446    3.73109    0.00000
Si    2.02582    0.68287    0.00000
Si    2.02252    4.19810    0.00000
Si    1.95193    0.20395    0.00000
Si    2.08428    1.51611    0.00000
Si    2.14445    1.22922    0.00000
Si    2.10184    2.21189    0.00000
Si    2.12094    2.66413    0.00000
Si    2.14538    3.92341    0.00000
Si    2.13691    1.91588    0.00000
Si    2.20100    2.96350    0.00000
Si    2.24561    4.43390    0.00000
Si    2.31107    0.62562    0.00000
Si    2.24218    4.74579    0.00000
Si    2.29142    1.68949    0.00000
Si    2.32682    3.39695    0.00000
Si    2.31145    2.43163    0.00000
Si    2.45255    0.37523    0.00000
Si    2.46138    1.13495    0.00000
Si    2.39750    3.10411    0.00000
Si    2.44607    3.86059    0.00000
Si    2.50842    0.82817    0.00000
```

Si	2.55515	3.58230	0.00000
Si	2.56846	4.36087	0.00000
Si	2.61831	1.65765	0.00000
Si	2.68072	1.35147	0.00000
Si	2.61913	2.44547	0.00000
Si	2.67517	4.06919	0.00000
Si	2.74566	2.73961	0.00000
Si	2.69084	3.04901	0.00000
Si	2.71273	4.63011	0.00000
Si	2.73423	0.39816	0.00000
Si	2.76966	0.69231	0.00000
Si	2.83398	3.52039	0.00000
Si	2.90001	1.78041	0.00000
Si	2.89160	2.29395	0.00000
Si	2.94734	3.22594	0.00000
Si	2.96293	1.28749	0.00000
Si	3.02172	2.01387	0.00000
Si	2.97407	4.03957	0.00000
Si	3.01945	0.29499	0.00000
Si	3.02627	3.74829	0.00000
Si	3.00943	4.57507	0.00000
Si	3.06263	0.75771	0.00000
Si	3.11150	1.03587	0.00000
Si	3.11883	4.29224	0.00000
Si	3.06862	1.55940	0.00000
Si	2.99141	2.57701	0.00000
Si	3.13972	4.83487	0.00000
Si	3.22679	3.11854	0.00000
Si	3.21724	0.52680	0.00000
Si	3.30056	2.06554	0.00000
Si	3.29596	2.62310	0.00000
Si	3.31851	3.64476	0.00000
Si	3.41404	2.32964	0.00000
Si	3.41382	3.34507	0.00000
Si	3.36933	1.60480	0.00000
Si	3.39192	2.90183	0.00000
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Si	3.41784	4.83640	0.00000
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Si	3.50218	1.86513	0.00000
Si	3.54731	4.58622	0.00000
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Si	3.60415	3.78417	0.00000
Si	3.64214	4.08418	0.00000
Si	3.69867	3.01398	0.00000
Si	3.73719	0.37150	0.00000
Si	3.70670	3.32453	0.00000
Si	3.73722	2.29870	0.00000
Si	3.78155	1.96976	0.00000

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Si    3.82781    1.35525    0.00000
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Si    3.93093    2.79381    0.00000
Si    3.84727    4.55525    0.00000
Si    3.91508    0.82562    0.00000
Si    3.87110    4.24971    0.00000
Si    4.01870    1.11631    0.00000
Si    4.05533    1.55067    0.00000
Si    4.00011    0.53722    0.00000
Si    4.05701    1.83451    0.00000
Si    4.11679    4.71934    0.00000
Si    4.11322    3.64459    0.00000
Si    4.23719    3.92245    0.00000
Si    4.18748    4.23978    0.00000
Si    4.21076    2.80853    0.00000
Si    4.20666    2.51916    0.00000
Si    4.33833    4.50837    0.00000
Si    4.28031    0.52169    0.00000
Si    4.32756    1.07160    0.00000
Si    4.35185    1.84081    0.00000
Si    4.40844    0.78191    0.00000
Si    4.37751    3.53507    0.00000
Si    4.33084    1.54231    0.00000
Si    4.44691    2.35159    0.00000
Si    4.45650    2.97116    0.00000
Si    4.51286    0.32909    0.00000
Si    4.50690    3.26557    0.00000
Si    4.53340    2.07256    0.00000
Si    4.51807    1.32189    0.00000
Si    4.48701    3.77937    0.00000
Si    4.62100    4.55432    0.00000
Si    4.68355    4.84758    0.00000
Si    4.70184    2.51007    0.00000
Si    4.69816    2.80793    0.00000
Si    4.70847    0.78420    0.00000
Si    4.78192    3.81791    0.00000
Si    4.82281    0.22978    0.00000
Si    4.82617    1.29387    0.00000
Si    4.80387    3.26751    0.00000
Si    4.84021    2.06918    0.00000
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O    0.68077    4.68082    0.00000
O    0.87942    4.88632    0.00000
O    1.10547    4.83152    0.00000
O    1.36577    4.72192    0.00000
O    1.16027    4.57807    0.00000
O    1.63292    4.67397    0.00000
O    1.88637    4.71507    0.00000
O    1.75622    4.46847    0.00000
O    2.24257    4.60547    0.00000
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O	2.62617	4.50957	0.00000
O	3.10567	4.69452	0.00000
O	3.28377	4.84522	0.00000
O	3.47557	4.71507	0.00000
O	3.69477	4.58492	0.00000
O	3.49612	4.44792	0.00000
O	3.27007	4.29037	0.00000
O	3.05087	4.42737	0.00000
O	2.63302	4.21502	0.00000
O	2.85907	4.60547	0.00000
O	2.41382	4.39997	0.00000
O	2.11927	4.31777	0.00000
O	1.88637	4.26982	0.00000
O	2.08502	4.05747	0.00000
O	1.63292	4.22187	0.00000
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O	1.16027	4.27667	0.00000
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O	0.79722	4.17392	0.00000
O	0.68077	3.92732	0.00000
O	0.94107	3.94787	0.00000
O	1.16712	4.02322	0.00000
O	1.09862	3.77662	0.00000
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O	1.59182	3.69442	0.00000
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O	1.60552	3.97527	0.00000
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O	4.66747	4.70137	0.00000
O	4.83872	4.20132	0.00000

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O    3.16732    3.70812    0.00000
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O    2.89332    3.37932    0.00000
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O    1.98227    3.29027    0.00000
O    1.95487    3.58482    0.00000
O    1.48222    3.41357    0.00000
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O    0.51637    3.70812    0.00000
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O    4.85242    3.13272    0.00000
O    4.49622    3.11217    0.00000
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O    2.90017    2.68747    0.00000
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O    1.74252    2.64637    0.00000
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O    1.01642    2.81762    0.00000
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O    0.74242    2.72857    0.00000
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O    1.68087    2.16002    0.00000
O    1.94802    2.23537    0.00000
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O    1.99597    2.57787    0.00000
O    2.22887    2.55732    0.00000
O    2.22202    2.31072    0.00000
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O    2.72892    2.33127    0.00000
O    2.98237    2.43402    0.00000
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O    3.74272    2.12577    0.00000
O    3.88657    2.38607    0.00000
O    4.23592    2.66007    0.00000
O    3.87972    2.66007    0.00000
O    4.06467    2.49567    0.00000
O    4.31127    2.42032    0.00000
O    4.46882    2.20112    0.00000
O    4.56472    2.44772    0.00000
O    4.68802    2.66007    0.00000
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O    3.93452    1.92027    0.00000
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O    3.95507    1.45447    0.00000
O    4.18797    1.50927    0.00000
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O    3.44817    1.46817    0.00000
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O    0.35882    1.00237    0.00000
O    0.11222    1.00237    0.00000
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O    3.12622    0.42697    0.00000
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O    3.91397    0.42697    0.00000
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O    3.48927    1.18732    0.00000
O    3.48927    0.92017    0.00000
O    3.90712    1.21472    0.00000
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O    4.40032    0.44752    0.00000
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- 500 particle coordinates from $T^* = 0.015$

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500
 Periodic Box, size = 49.17 X 49.17 X 0.0, 200 Si and 300 O particles
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  Si         1.421330       22.181200        0.000000
  Si        19.133400       28.823000        0.000000
  Si        34.500500       24.775900        0.000000
  Si        26.178600       40.722099        0.000000
  Si        42.705502       46.093899        0.000000
  Si        47.313900       14.420500        0.000000
  Si        30.010500       44.909698        0.000000
  Si        28.015200        5.861840        0.000000
  Si        21.608101        9.767880        0.000000
  Si         3.879510        3.589230        0.000000
  Si        25.176100        6.888140        0.000000
  Si        12.700600       34.073700        0.000000
  Si        35.657398        7.245140        0.000000
  Si        33.008202       12.105300        0.000000
  Si        47.231800       27.637100        0.000000
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Si	15.737900	0.297935	0.000000
Si	15.213800	43.925201	0.000000
Si	31.036800	15.559600	0.000000
Si	16.760300	30.722799	0.000000
Si	17.711901	2.637900	0.000000
Si	47.376801	2.515360	0.000000
Si	44.904598	25.678801	0.000000
Si	46.929699	38.000500	0.000000
Si	6.126490	38.522598	0.000000
Si	13.164300	26.410500	0.000000
Si	12.390300	16.249399	0.000000
Si	10.770700	41.765900	0.000000
Si	31.760300	23.503700	0.000000
Si	41.830799	2.547890	0.000000
Si	12.867700	19.268299	0.000000
Si	27.174999	43.664600	0.000000
Si	0.749167	9.708330	0.000000
Si	32.085499	40.216599	0.000000
Si	30.589600	34.781898	0.000000
Si	22.664101	19.505301	0.000000
Si	44.694500	22.647301	0.000000
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Si	23.109800	24.785500	0.000000
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Si	17.987301	26.005899	0.000000
Si	38.418301	47.777100	0.000000
Si	15.298200	7.591830	0.000000
Si	15.170900	14.981000	0.000000
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Si	42.139999	10.803900	0.000000
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Si	22.026199	45.074902	0.000000
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Si	30.624701	18.530899	0.000000
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Si	22.098400	29.598900	0.000000
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Si	27.347099	11.468700	0.000000
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Si	10.291800	7.214740	0.000000

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Notes and references

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