Supplementary Information
for
Al-Driven Cement Functionality by Manifold Structuring & Disorder

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Contents	**Page**

3D Volume Calculator

The 3-dimensional (3D) volume of the models can be computed through multiplying three orthogonal axes that approximate the largest extant of the space occupied by the cement nano-particle. Alternatively, the volume can be computed from a series of polyhedral. The concept of calculating volumes from coordinates is deeply rooted in geometry and applied mathematics. In computational geometry, the volume of 3D shapes, such as tetrahedra or polyhedra, can be derived using determinants. This technique is widely used in CAD software, physics simulations, and geographic modelling. For arbitrary polyhedral – such as the cement nano-particles, the total volume is the sum of the volumes of individual tetrahedra formed by connecting vertices to a common reference point.

See: 3-D volume Calculator for Arbitrary Coordinates:
https://www.calculatorultra.com/en/tool/3d-volume-calculator-arbitrary-coordinates.html#google_vignette

Quantum Chemical Confirmation of Pore Stability

Towards further determining the stability of the cement nano-clusters the final geometry of structures emerging from NPT and NVE production runs, were subjected to quantum chemical electronic structure computations, employing the HF/3-21G ab initio method. The resultant geometry-optimised structures required quite a lengthy process, including a large number of iterations, which were subsequently confirmed as residing at minima on their respective potential energy hypersurfaces (PEHSs). The structure shown in **Figure S1** is 244 atom cement nano-clusters ($Ca_{34}Al_2Si_{22}H_{70}O_{116}$), with a porosity of ~11%, arising from the pore and total volumes of ~0.625nm^3 and ~5.6nm^3, respectively (where 0.625/5.600 ≈ 0.1116), matching well with established values in the literature.[Refs S1-S2].

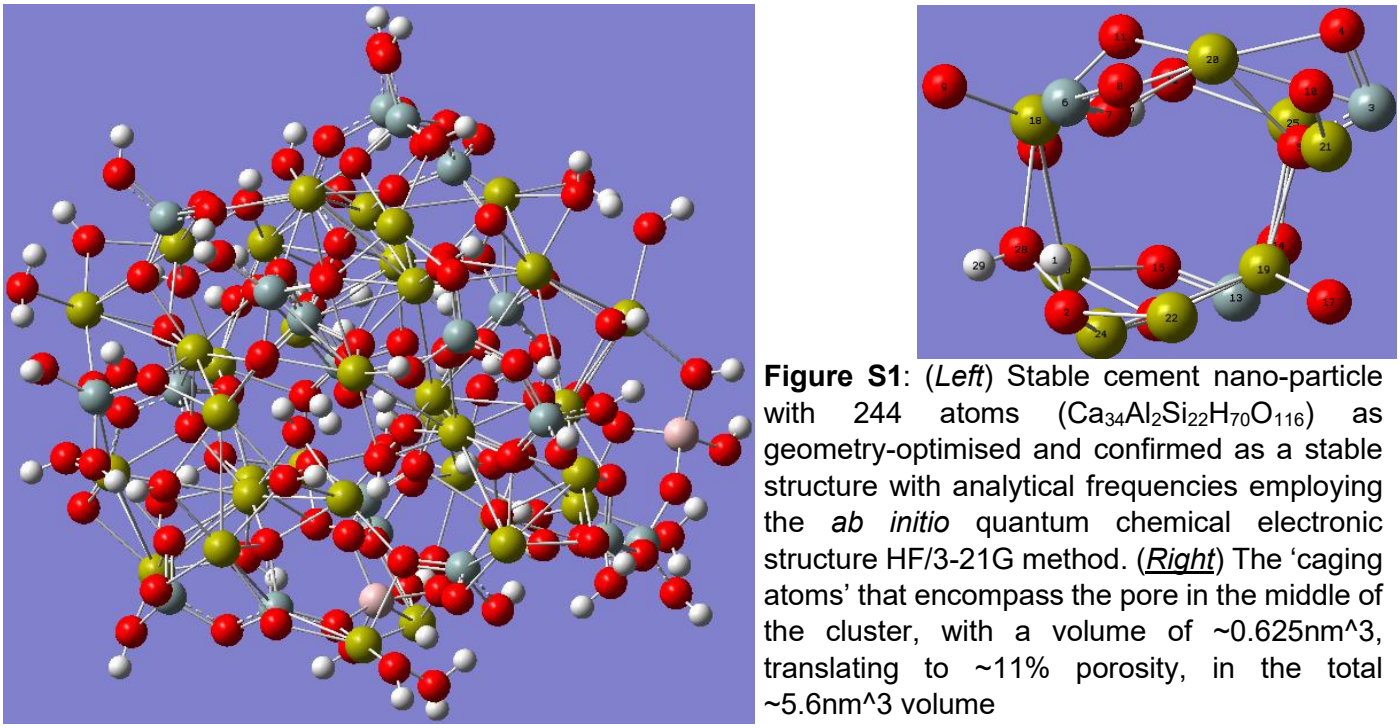

Figure S1: (*Left*) Stable cement nano-particle with 244 atoms ($Ca_{34}Al_2Si_{22}H_{70}O_{116}$) as geometry-optimised and confirmed as a stable structure with analytical frequencies employing the *ab initio* quantum chemical electronic structure HF/3-21G method. (*Right*) The 'caging atoms' that encompass the pore in the middle of the cluster, with a volume of ~0.625nm^3, translating to ~11% porosity, in the total ~5.6nm^3 volume

Regarding the HF/3-21G method, albeit not for determination of energetics, electron densities, electronic properties or properties, it is surprisingly robust in geometry predictions. Such a 'fortuitous cancellation of errors', this method has been shown to be a reliable means to structure predictions, for example for initial structural; guesses as well as in large conformational searching – with geometries very similar to those generated with post-HF methods and more complete basis sets (Ex. MP2/6-31G(d) and beyond), and matching well with experimentally-determined structures – for a myriad of differing systems (from ordered materials, and lanthanide-containing compounds to peptides and beyond).[Refs S3-S9]

References: **S1)** C. Li, et. al., *Materials*, 2022, 15, 112; **S2)** W. Sekkal, *Cem. Conc. Res.*, 2016, 87, 45–52; **S3)** K.E. Riley, et. al., *J Chem Theory Comput.*, 2007; 3(2): 407–433; **S4)** N. Chen, et. al., *Ind. Eng. Chem. Res.,* 1996**,** *35,* 4020-4027; **S5)** N.U. Zhanpeisov, *Res. Chem. Intermed.,* 2021, 47:157–168; **S6)** V. A. Karttunen, et. al., *Theor Chem Accounts*, 2007, 118:899–913; **S7)** J. Nagy, et. al., *J. Org. Chem.*, 1998, 63, 5824-5830; **S8)** G. Endredi, et. al., *J. Mol. Struct. (Theochem)*, 1997, 391, 15-26; **S9)** I. A. Topol, et. al., *J. Am. Chem. Soc.*, 2001, 123, 25, 6054–6060

Model	Al-co	Al Q	%Q0	%Q1	%Q2	%Q3
Order	-	-	12.50	45.83	33.33	8.33
Disorder	-	-	8.33	66.67	25.00	0.00
D_P	-	-	8.33	66.67	25.00	0.00
D_H_P	-	-	16.67	58.33	25.00	0.00
O_L	Al5 Al5	2Q3	4.17	75.00	20.83	8.33
O_N	Al4 Al4	2Q3	4.17	75.00	20.83	8.33
D_L	Al4 Al5	2Q2	8.33	66.67	25.00	0.00
D_N	Al4 Al6	2Q2	4.17	66.67	29.17	0.00
D_P_L	Al4 Al5	2Q2	8.33	66.67	25.00	0.00
D_P_N	Al4 Al5	2Q2	12.50	70.83	16.67	4.17
D_H_L	Al4 Al4	2Q2	16.67	58.33	25.00	0.00
D_H_N	Al4 Al4	2Q2	8.33	66.67	25.00	0.00
O_L	6 Al4	Q1 3Q2 Q3	8.33	50.00	41.67	0.00
O_A_N	6 Al4	2Q1 4Q2	12.50	58.33	29.17	0.00
D_L	3 Al4 3 Al5	2Q1 3Q2 1Q3	8.70	60.87	30.43	4.35
D_N	4 Al4 Al5 Al6	Q1 5Q2	12.50	58.33	20.83	8.33
D_P_L	2 Al4 4 Al5	3Q1 3Q2	8.33	66.67	25.00	0.00
D_P_N	6 Al4	Q1 5Q2	12.50	66.67	20.83	0.00
D_H_L	3 Al5, 3 Al4	3Q1 3Q2	8.33	66.67	25.00	0.00
D_H_N	5 Al4 Al5	6Q2	8.33	66.67	25.00	0.00

Table S1. Analysis of Al coordination, Al Q number and the overall proportions of Q0, Q1, Q2 and Q3 Al + Si present in each model. Models that conform to the ideal Qn ratio for C-S-H given by NMR are highlighted in green. O = Order, D = Disorder, P = Pore, H_P = Hydrated Pore, L = Loewenstein, N = No Loewenstein.

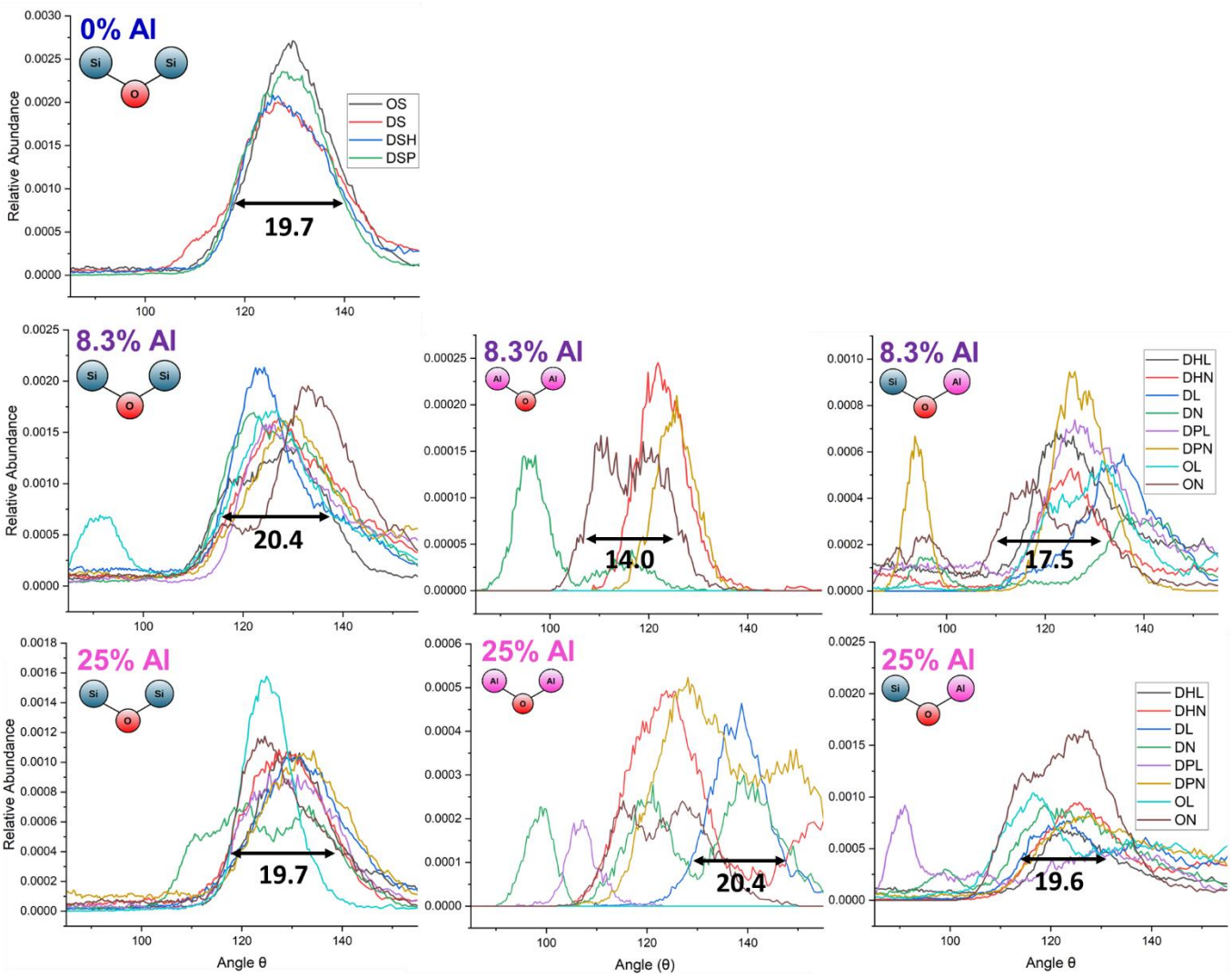

Figure S2. ADFs the angles about the oxygen atoms, Si-O-Si, Al-O-Al and Si-O-Al. FWHMs shown are averages for all angles of each set. D = Disorder, H = Hydrated pore, L = Loewenstein (Al avoidance), N = No Loewenstein (No Al avoidance), O = Order, S = Silicon (No Al present).

O-Al-O	highal_hydropore_lo	highal_hydro_nolo	highal_lo	highal_nolo	highal_pore_lo	highal_pore_nolo	order_highal_lo	order_highal_nolo	Average
STDEV	8.7	11.6	25.1	10.9	12.1	8.7	8.2	7.8	
FWHM	20.6	27.2	59.2	25.6	28.5	20.6	19.5	18.5	**27.4625**
	al_hydropore_lo	al_hydro_nolo	al_lo	al_nolo	al_pore_lo	al_pore_nolo	order_al_lo	order_al_nolo	
STDEV	7.4	12.5	10.2+5.6+3.23	18.65	48.95	5+3.43	9.5	8.16	
FWHM	17.4	29.5	24.2+13.3+7.6	43.97	115.3	11.8+8	22.4	19.2	**41.295**
	disorder_si_hydro	disorder_si	disorder_si_pore	order_si					
STDEV	-	-	-	-					
FWHM	-	-	-	-					
O-Si-O	highal_hydropore_lo	highal_hydro_nolo	highal_lo	highal_nolo	highal_pore_lo	highal_pore_nolo	order_highal_lo	order_highal_nolo	
STDEV	6.2	5.65	6	5.65	5.56	6.32	3.19	5.89	
FWHM	14.6	13.3	14.1	13.3	13.3	14.88	13.19	13.86	**13.81625**
	al_hydropore_lo	al_hydro_nolo	al_lo	al_nolo	al_pore_lo	al_pore_nolo	order_al_lo	order_al_nolo	
STDEV	6.14	7.22	6.33	6.14	6.1	6.35	5.42	6.78	
FWHM	14.4	17.07	14.9	14.47	14.36	14.97	15.1	15.97	**15.155**
	disorder_si_hydro	disorder_si	disorder_si_pore	order_si					
STDEV	6.04	6.4	6.5	6					
FWHM	14.22	15	15.34	14.1					**14.665**
Al-O-Al	highal_hydropore_lo	highal_hydro_nolo	highal_lo	highal_nolo	highal_pore_lo	highal_pore_nolo	order_highal_lo	order_highal_nolo	
STDEV	-	7+10.2	5.34	5.76+4.9+2.74	2.76	16.48	-	9.98	
FWHM	-	16.47+24.0	12.6	13.56+11.57+6.56	6.5	38.8	-	23.5	**20.35**
	al_hydropore_lo	al_hydro_nolo	al_lo	al_nolo	al_pore_lo	al_pore_nolo	order_al_lo	order_al_nolo	
STDEV	-	4.82	-	3.2+5.8	-	4.11	-	8.9	
FWHM	-	11.36	-	7.6+13.8	-	9.69	-	20.9	**13.98333333**
	disorder_si_hydro	disorder_si	disorder_si_pore	order_si					
STDEV	-	-	-	-					
FWHM	-	-	-	-					
Si-O-Si	highal_hydropore_lo	highal_hydro_nolo	highal_lo	highal_nolo	highal_pore_lo	highal_pore_nolo	order_highal_lo	order_highal_nolo	
STDEV	7.48	7.85	8.9	13.7	8.9	8.3	4.8	7	
FWHM	17.58	18.5	21.03	32.4	21.1	19.56	11.26	16.51	**19.7425**
	al_hydropore_lo	al_hydro_nolo	al_lo	al_nolo	al_pore_lo	al_pore_nolo	order_al_lo	order_al_nolo	
STDEV	10.69	10.1	5.3	10.97	8.12	8.4	7.8+3.72	7.1	
FWHM	25.2	23.7	12.4	25.8	19.13	19.7	18.41+8.76	16.7	**20.37571429**
	disorder_si_hydro	disorder_si	disorder_si_pore	order_si					
STDEV	8.1	9.69	7.9	7.8					
FWHM	19.1	22.8	18.69	18.45					**19.76**
Si-O-Al	highal_hydropore_lo	highal_hydro_nolo	highal_lo	highal_nolo	highal_pore_lo	highal_pore_nolo	order_highal_lo	order_highal_nolo	
STDEV	6.72	7.4	5.57	9.82	2.03+8.33	14.7	4.4	9.62	
FWHM	15.8	17.42	13.1	23.13	4.8+19.6	34.7	10.3	22.66	**19.58714286**
	al_hydropore_lo	al_hydro_nolo	al_lo	al_nolo	al_pore_lo	al_pore_nolo	order_al_lo	order_al_nolo	
STDEV	6.8	5.7	8.2	6.42	6.92	5.34+5.30	8.56	9.31	
FWHM	15.9	13.45	19.31	15.13	16.29	12.58+12.52	20.16	21.92	**17.45142857**
	disorder_si_hydro	disorder_si	disorder_si_pore	order_si					
STDEV	-	-	-	-					
FWHM	-	-	-	-					

Table S2. Standard deviations and full width half maxima for each peak corresponding to angles of type (top) O-Al-O, O-Si-O, Al-O-Al, Si-O-Si, Si-O-Al (bottom) for each model. + is used to indicate where one model has multiple peaks for the same angle e.g. al_pore_nolo **12.58+12.52**. Averages collected in the last column

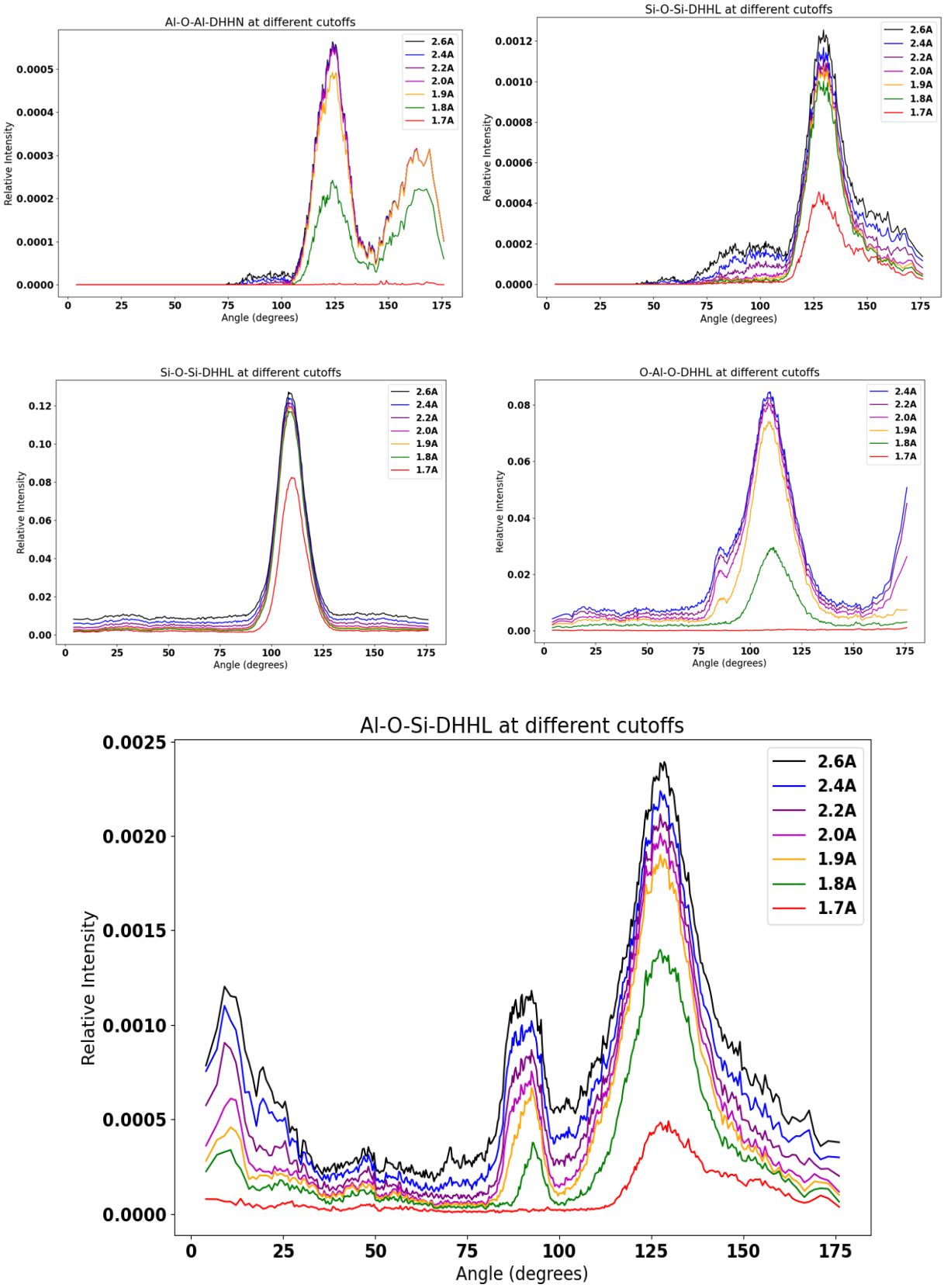

Figure S3. Visualisation of ADFs for 25% Al Disordered Hydropore/Saturated Pore Lo at different radial cutoffs. Any angles found outside the cutoff threshold from the origin are not included in the data. E.g., where the origin point for Al-O-Al is the O atom, any bond angles > 2.4A away from the origin are excluded from the data. In the study 1.9A was chosen as the minimum cutoff that preserved the most information.

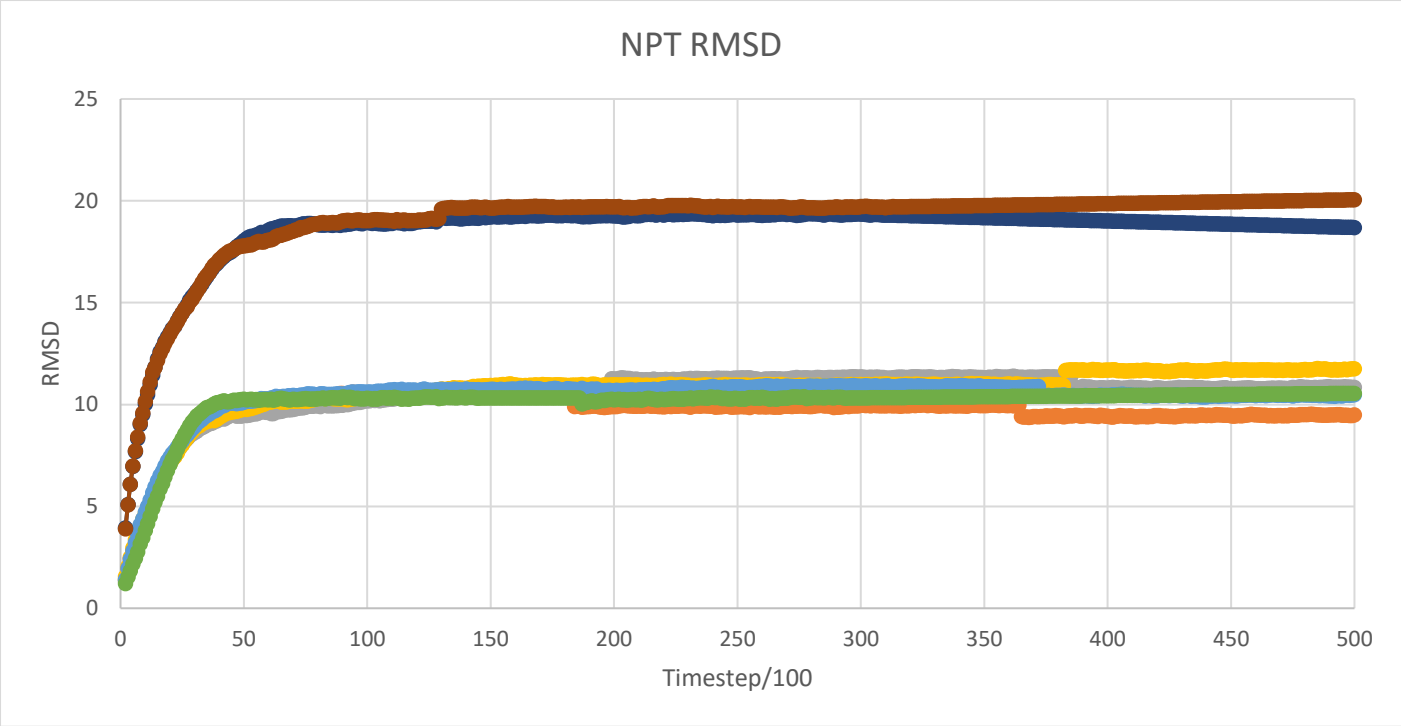

Figure S4. RMSD for 33% Al NPT runs. Jumps in RMSD from 100 steps onward are due to restarting the trajectories from input files where the restart files could not be used. Each step is 0.25fs for a total duration of 125ps of NPT.

Final NVE Geometries

33% Al

Disorder Hydrated Pore L_w

HEADER CSD ENTRY i = 25000, time = 25000.000, E = -3245.3136659209
CRYST1 1.0000 1.0000 1.0000 90.00 90.00 90.00
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Disorder Hydrated Pore

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Disorder Hydrated Pore

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Disorder Si Hydrated Pore

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