Supplementary Information for:

Computational Characterisation of Dried and Hydrated Graphene Oxide Membranes

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1. Parameters for GO Flake Atoms

Figure S1 shows the GO flake atom types, Table S1 the non-bonded interaction parameters and Table S2 the bonded interaction parameters. The CHARMM force field was used for all interaction parameters.

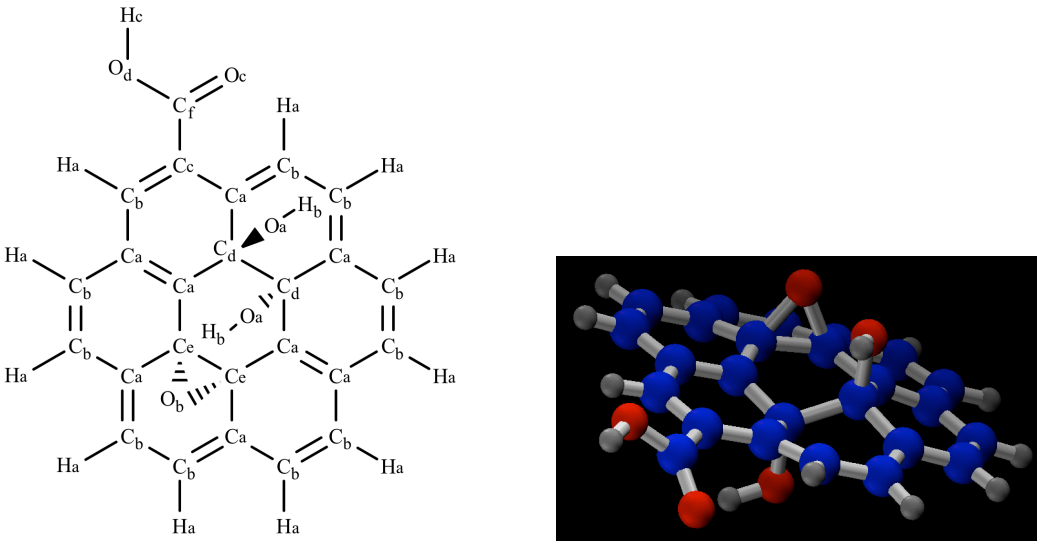

Figure S1. GO flake model with non-bonded atom types corresponding to Table 1.

i	σ_i (nm)	ε_i (kJ mol^{-1})	q_i (*e*)
C_a	0.355005	0.29288	0.000
C_b	0.355005	0.29288	−0.158
C_c	0.355005	0.29288	0.066
C_d	0.356359	0.13389	0.263
C_e	0.358141	0.23430	0.184
C_f	0.302906	0.41003	0.723
O_a	0.314487	0.80375	−0.661
O_b	0.293997	0.41840	−0.368
O_c	0.302906	0.50208	−0.585
O_d	0.314487	0.80375	−0.640
H_a	0.242003	0.12552	0.158
H_b	0.040001	0.19246	0.398
H_c	0.040001	0.19246	0.436

Table S1. Non-bonded parameters for GO flakes.

Bonds

i	*j*	r_{eq} (nm)	k_r (kJ mol^{-1} nm^{-2})
$C_{a/b/c}$	$C_{a/b/c}$	0.1375	255224.0
$C_{a/b/c}$	$C_{d/e}$	0.1490	192464.0
C_c	C_f	0.1480	212547.2
$C_{a/b/c}$	H_a	0.1080	284512.0
C_d	C_d	0.1500	186188.0
C_d	C_e	0.1500	230120.0
C_d	O_a	0.1420	358150.4
C_e	C_e	0.1501	200832.0
C_e	O_b	0.1450	184096.0
C_f	O_c	0.1220	627600.0
C_f	O_d	0.1400	192464.0
$O_{a/d}$	$H_{b/c}$	0.0960	456056.0

Angles

i	*j*	*k*	θ_{eq} (degrees)	k_θ (kJ mol^{-1} rad^{-2})	r_u (nm)	k_u (kJ mol^{-1} nm^{-2})
$C_{a/b/c}$	$C_{a/b/c}$	$C_{a/b/c}$	120.0	334.720	0.24162	29288.0
$C_{a/b/c}$	$C_{a/b/c}$	$C_{d/e}$	120.0	383.254	-	-
$C_{a/b/c}$	$C_{a/b/c}$	C_f	120.0	376.560	-	-
$C_{a/b/c/d/e}$	$C_{a/b/c}$	H_a	120.0	251.040	0.21525	18409.6
H_a	$C_{a/b/c}$	H_a	110.1	221.752	0.21790	18853.1
$C_{a/b/c}$	C_d	$C_{a/b/c/d}$	107.5	433.462	-	-
$C_{a/b/c}$	C_d	O_a	110.1	633.458	-	-
C_d	C_d	O_a	111.5	376.560	-	-
$C_{d/e}$	C_d	$C_{d/e}$	113.6	488.273	0.25610	9338.69
$C_{a/b/c/d/e}$	C_e	O_b	103.0	251.040	-	-
$C_{a/b/c}$	C_f	O_c	123.1	585.760	0.24420	16736.0
$C_{a/b/c}$	C_f	O_d	113.9	334.720	0.23700	25104.0
$O_{c/d}$	C_f	$O_{c/d}$	123.0	418.400	0.22620	175728.0
C_d	O_a	H_b	106.0	418.400	-	-
C_f	O_d	H_b	115.0	460.240	-	-
C_e	O_b	C_e	97.0	421.329	-	-

Dihedrals

i	*j*	*k*	*l*	ϕ_{eq} (degrees)	*n*	k_ϕ (kJ mol^{-1} rad^{-2})
$C_{a/b/c/d/e/f}$	$C_{a/b/c}$	$C_{a/b/c}$	$C_{a/b/c/d/e/f}$	180.0	2	12.97040
$C_{a/b/c/d/e/f}$	$C_{a/b/c}$	$C_{a/b/c}$	H_a	180.0	2	17.57280
H_a	$C_{a/b/c}$	$C_{a/b/c}$	H_a	180.0	2	10.04160
$C_{a/b/c}$	$C_{a/b/c}$	C_d	$C_{a/b/c/d/e/f}$	180.0	3	0.16736
$C_{a/b/c/d/e}$	$C_{a/b/c}$	C_f	O_c	180.0	2	4.28860
$C_{a/b/c/d/e}$	C_d	C_d	$C_{a/b/c/d/e}$	0.0	3	0.83680
$C_{a/b/c/d}$	$C_{a/b/c/d}$	C_d	O_b	180.0	1	1.96648
H_a	$C_{a/b/c}$	C_d	O_b	0.0	1	2.09200
$C_{a/b/c/d/e}$	C_e	C_e	O_b	180.0	6	0.46024
$C_{a/b/c/d}$	C_d	O_a	H_b	0.0	1	4.72792
$C_{a/b/c}$	C_f	O_a	H_b	180.0	2	8.57720

Table S2. Bonded parameters for GO flakes.

2. Finite Flake-Size Effects

The size of GO flakes used in the simulations is limited by computational cost. Consequently, the flakes are much smaller than those in a real GO membrane, which have sizes ~ μm. To investigate the possibility of finite flake size effects, L was varied between 3 nm and 9 nm. The interlayer distance, d, decreases rapidly when L is increased from 3 nm to 5 nm, but converges beyond 5 nm (Figure S2). The initial decrease is due to small discrepancies between L and the size of the GO flakes (chosen to match L as closely as possible), which are not exactly equal both due to the underlying hexagonal structure and edge-functionalisation of the flakes. This effect diminishes with increasing flake size because the ratio of the GO flake area to L^2 converges with increasing simulation size. The data for all of these models are provided in Tables S3 – S9.

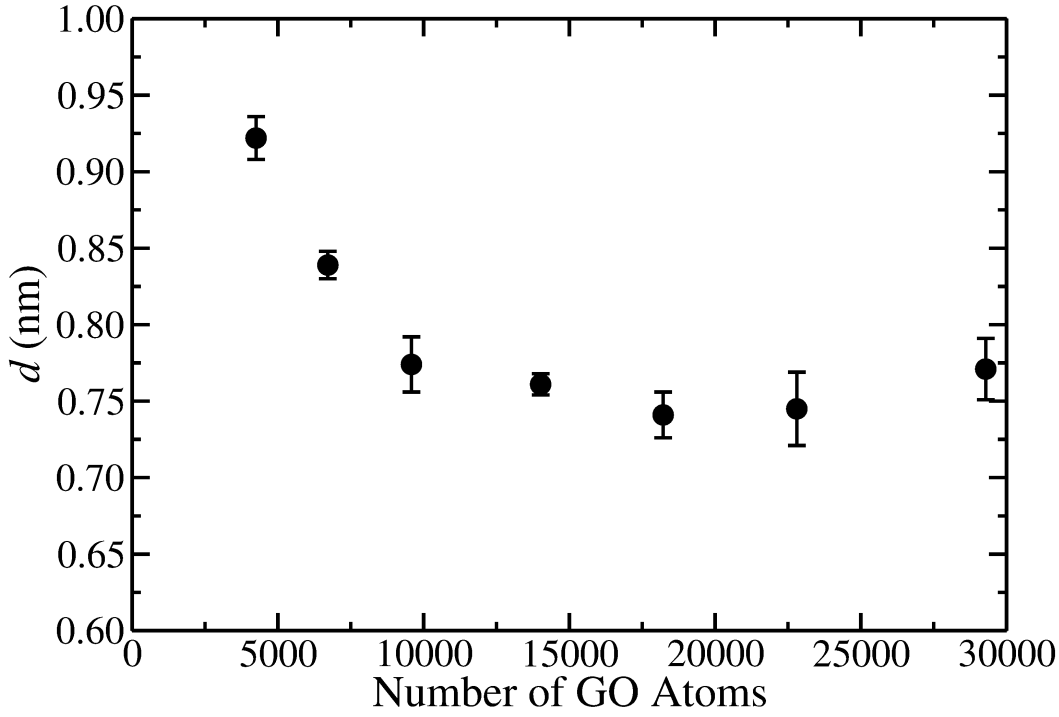

Figure S2 Variation of interlayer distance, d, with GO flake size for membranes prepared without water (GO-L-0-d-s).

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	4290	25.0	0.0	0.480	0.932	0.175	165.7	0.320	1.58
2	4230	25.1	0.0	0.474	0.861	0.107	111.0	0.280	1.69
3	4170	25.1	0.0	0.469	0.914	0.180	188.4	0.343	1.58
4	4398	25.2	0.0	0.489	0.984	0.199	233.2	0.412	1.53
5	4206	25.1	0.0	0.469	0.884	0.135	104.8	0.310	1.63
6	4332	25.0	0.0	0.478	0.981	0.212	174.8	0.417	1.50
7	4188	25.1	0.0	0.476	0.885	0.138	103.9	0.376	1.66
8	4326	25.0	0.0	0.485	0.898	0.131	74.2	0.270	1.66
9	4224	25.0	0.0	0.467	0.887	0.146	82.4	0.317	1.62
10	4134	25.1	0.0	0.468	0.990	0.225	286.7	0.946	1.46
Mean	4250	25.1	0.0	0.476	0.922	0.165	152.4	0.399	1.59
Error	-	-	-	-	0.014	0.019	38.2	0.118	0.04

Table S3. GO-3-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	6630	25.2	0.0	0.749	0.776	0.127	74.6	0.402	1.67
2	6720	25.1	0.0	0.763	0.832	0.179	207.0	0.450	1.59
3	6642	25.1	0.0	0.755	0.851	0.204	241.9	0.720	1.54
4	6824	25.0	0.0	0.762	0.854	0.200	296.1	0.522	1.55
5	6732	25.1	0.0	0.764	0.860	0.194	258.9	0.834	1.54
6	6756	25.1	0.0	0.769	0.814	0.159	107.3	0.330	1.63
7	6666	25.0	0.0	0.751	0.825	0.180	173.5	0.341	1.58
8	6720	25.1	0.0	0.763	0.849	0.254	215.0	0.351	1.56
9	6666	25.1	0.0	0.756	0.847	0.202	272.1	0.376	1.54
10	6798	25.0	0.0	0.767	0.884	0.220	357.7	0.419	1.50
Mean	6715	25.1	0.0	0.760	0.839	0.192	220.4	0.475	1.57
Error	-	-	-	-	0.009	0.010	25.6	0.052	0.02

Table S4. GO-4-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.834	0.239	242.9	0.766	1.45
2	9678	25.1	0.0	1.109	0.906	0.302	383.9	0.842	1.36
3	9630	25.1	0.0	1.092	0.756	0.171	208.0	0.347	1.60
4	9444	25.1	0.0	1.068	0.717	0.153	127.9	0.283	1.65
5	9486	25.1	0.0	1.087	0.749	0.175	70.8	0.522	1.61
6	9510	25.1	0.0	1.071	0.730	0.165	142.6	0.345	1.62
7	9516	25.1	0.0	1.080	0.729	0.149	158.7	0.369	1.64
8	9516	25.1	0.0	1.090	0.826	0.234	344.4	0.889	1.46
9	9642	25.0	0.0	1.094	0.751	0.166	184.7	0.290	1.61
10	9768	25.0	0.0	1.112	0.743	0.143	147.1	0.405	1.66
Mean	9581	25.1	0.0	1.090	0.774	0.190	201.1	0.506	1.57
Error	-	-	-	-	0.018	0.016	29.4	0.071	0.03

Table S5. GO-5-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	14010	25.0	0.0	1.599	0.747	0.156	183.1	0.371	1.65
2	13836	25.0	0.0	1.590	0.749	0.159	132.7	0.421	1.63
3	14082	25.1	0.0	1.612	0.766	0.175	202.4	0.489	1.62
4	13896	25.1	0.0	1.584	0.738	0.159	231.0	0.414	1.65
5	14262	25.0	0.0	1.629	0.765	0.165	164.2	0.429	1.64
6	13908	25.0	0.0	1.591	0.730	0.143	161.0	0.326	1.68
7	14196	25.0	0.0	1.612	0.762	0.170	188.6	0.488	1.63
8	13986	25.0	0.0	1.609	0.760	0.161	79.1	0.334	1.63
9	14106	25.0	0.0	1.603	0.809	0.217	334.7	0.540	1.52
10	13848	25.0	0.0	1.595	0.784	0.195	283.3	0.680	1.57
Mean	14013	25.0	0.0	1.602	0.761	0.170	201.1	0.449	1.62
Error	-	-	-	-	0.007	0.008	23.9	0.030	0.01

Table S6. GO-6-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	18186	25.0	0.0	2.080	0.746	0.191	289.7	0.495	1.57
2	18174	25.0	0.0	2.080	0.789	0.236	312.3	0.968	1.49
3	18270	25.1	0.0	2.094	0.732	0.172	218.0	0.620	1.62
4	18258	25.0	0.0	2.086	0.716	0.165	145.1	0.444	1.65
5	18324	25.1	0.0	2.107	0.710	0.146	211.4	0.363	1.68
6	18204	25.0	0.0	2.109	0.719	0.161	208.0	0.409	1.66
7	18138	25.0	0.0	2.091	0.836	0.269	405.1	1.093	1.41
8	18258	25.0	0.0	2.107	0.681	0.121	0.0	0.264	1.75
9	18264	25.1	0.0	2.087	0.687	0.132	23.3	0.263	1.72
10	18126	25.0	0.0	2.075	0.797	0.239	346.3	1.085	1.47
Mean	18220	25.1	0.0	2.092	0.741	0.183	215.9	0.600	1.60
Error	-	-	-	-	0.015	0.015	39.5	0.098	0.03

Table S7. GO-7-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	22812	25.0	0.0	2.622	0.823	0.299	482.9	1.170	1.38
2	22824	25.0	0.0	2.635	0.686	0.157	229.3	0.500	1.66
3	22854	25.0	0.0	2.649	0.748	0.220	165.3	0.760	1.53
4	23064	25.0	0.0	2.642	0.689	0.157	115.5	0.383	1.66
5	22716	25.0	0.0	2.611	0.681	0.153	185.0	0.400	1.66
6	22944	25.0	0.0	2.633	0.789	0.257	417.7	0.756	1.44
7	22710	25.0	0.0	2.607	0.645	0.124	122.4	0.239	1.75
8	22758	25.0	0.0	2.619	0.887	0.352	483.2	1.470	1.28
9	22584	25.1	0.0	2.613	0.692	0.168	156.9	0.698	1.63
10	22770	25.0	0.0	2.614	0.809	0.279	356.9	1.276	1.40
Mean	22804	25.0	0.0	2.624	0.745	0.217	271.5	0.765	1.54
Error	-	-	-	-	0.020	0.019	44.5	0.125	0.04

Table S8. GO-8-0-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	29112	25.0	0.0	3.361	0.857	0.318	471.3	1.421	1.34
2	29244	25.0	0.0	3.397	0.754	0.215	293.7	0.802	1.54
3	29418	25.0	0.0	3.385	0.770	0.230	383.6	0.754	1.50
4	29268	25.0	0.0	3.373	0.777	0.238	359.0	1.152	1.48
5	29460	25.0	0.0	3.399	0.873	0.329	472.4	1.397	1.33
6	29676	25.0	0.0	3.410	0.708	0.166	141.2	0.461	1.65
7	29142	25.0	0.0	3.369	0.704	0.171	250.8	0.701	1.63
8	29376	25.0	0.0	3.382	0.704	0.162	142.8	0.448	1.64
9	29190	25.0	0.0	3.368	0.722	0.182	195.8	0.596	1.59
10	28962	25.0	0.0	3.348	0.838	0.297	422.1	1.386	1.37
Mean	29284	25.0	0.0	3.379	0.771	0.231	313.3	0.909	1.51
Error	-	-	-	-	0.020	0.019	38.2	0.118	0.04

Table S9. GO-9-0-d-s.

3. Rate of GO Flakes Pulling

Different rates of GO flake centre-of-mass pulling to $z = 0$ in step III were also investigated, but no significant differences in the membrane structures were observed for rates less than 0.01 nm ps^{-1}. All further GO membrane models were therefore prepared using a pulling rate of 0.01 nm ps^{-1}.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.761	0.163	172.8	0.399	1.59
2	9678	25.1	0.0	1.109	0.898	0.306	568.5	0.700	1.37
3	9630	25.1	0.0	1.092	0.750	0.168	207.8	0.695	1.61
4	9444	25.1	0.0	1.068	0.737	0.173	194.5	0.550	1.61
5	9486	25.1	0.0	1.087	0.721	0.150	120.9	0.347	1.67
6	9510	25.1	0.0	1.071	0.811	0.249	375.2	0.905	1.46
7	9516	25.1	0.0	1.080	0.745	0.171	212.7	0.365	1.61
8	9516	25.1	0.0	1.090	0.792	0.208	313.1	0.505	1.53
9	9642	25.0	0.0	1.094	0.803	0.280	340.7	0.745	1.51
10	9768	25.0	0.0	1.112	0.751	0.154	213.9	0.351	1.64
Mean	9581	25.1	0.0	1.090	0.777	0.202	272.0	0.556	1.56
Error	-	-	-	-	0.015	0.017	39.3	0.059	0.03

Table S10. GO-5-0-d-s prepared with a pulling rate in step III of 0.002 nm ps^{-1}.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.760	0.178	233.0	0.485	1.59
2	9678	25.1	0.0	1.109	0.806	0.219	327.7	0.631	1.52
3	9630	25.1	0.0	1.092	0.748	0.175	218.4	0.423	1.62
4	9444	25.1	0.0	1.068	0.750	0.189	252.4	0.537	1.58
5	9486	25.1	0.0	1.087	0.794	0.223	329.7	0.738	1.52
6	9510	25.1	0.0	1.071	0.779	0.223	369.0	0.479	1.52
7	9516	25.1	0.0	1.080	0.732	0.161	144.0	0.283	1.64
8	9516	25.1	0.0	1.090	0.715	0.130	154.1	0.386	1.69
9	9642	25.0	0.0	1.094	0.795	0.211	302.3	0.725	1.52
10	9768	25.0	0.0	1.112	0.820	0.226	323.0	0.330	1.50
Mean	9581	25.1	0.0	1.090	0.770	0.194	265.4	0.502	1.57
Error	-	-	-	-	0.010	0.010	23.2	0.047	0.02

Table S11. GO-5-0-d-s prepared with a pulling rate in step III of 0.005 nm ps^{-1}.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.745	0.163	220.4	0.442	1.62
2	9678	25.1	0.0	1.109	0.855	0.259	459.5	0.507	1.44
3	9630	25.1	0.0	1.092	0.722	0.144	62.4	0.226	1.68
4	9444	25.1	0.0	1.068	0.740	0.178	207.0	0.258	1.60
5	9486	25.1	0.0	1.087	0.705	0.123	123.6	0.330	1.71
6	9510	25.1	0.0	1.071	0.737	0.174	208.0	0.395	1.61
7	9516	25.1	0.0	1.080	0.716	0.139	34.9	0.468	1.67
8	9516	25.1	0.0	1.090	0.729	0.150	167.1	0.298	1.66
9	9642	25.0	0.0	1.094	0.781	0.202	310.7	0.819	1.55
10	9768	25.0	0.0	1.112	0.788	0.193	303.1	0.596	1.56
Mean	9581	25.1	0.0	1.090	0.752	0.173	209.7	0.434	1.61
Error	-	-	-	-	0.013	0.012	37.8	0.053	0.02

Table S12. GO-5-0-d-s prepared with a pulling rate in step III of 0.05 nm ps^{-1}.

4. GO Membrane Models Prepared with Water

Data for all hydrated GO membrane models is provided in Tables S13 – S20. Figure S3 shows that the presence of water does not reduce the propensity of GO flakes to aggregate during step III.

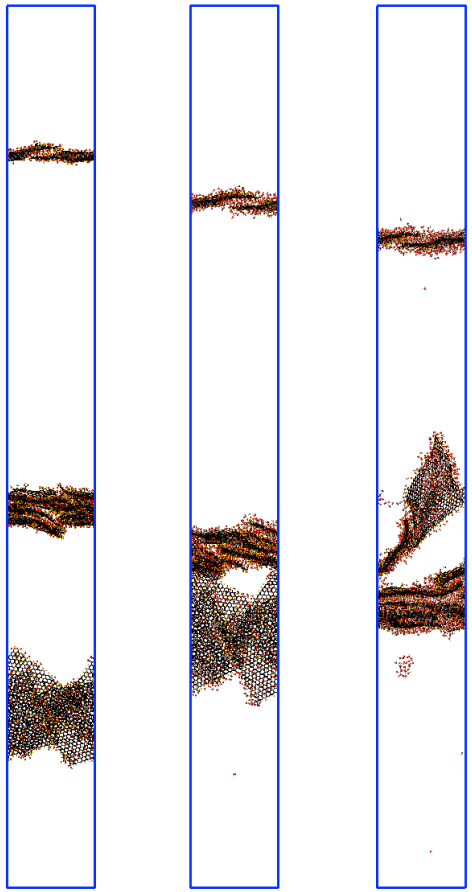

Figure S3. Aggregation of GO flakes during step III (at 0.5 ns) using the same starting configuration for GO flakes but with 0% (left), 10% (centre) and 20% (right) water content.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.751	0.166	200.0	0.444	1.61
2	9678	25.1	0.0	1.109	0.757	0.162	239.7	0.387	1.62
3	9630	25.1	0.0	1.092	0.762	0.175	214.3	0.605	1.59
4	9444	25.1	0.0	1.068	0.706	0.136	120.7	0.316	1.68
5	9486	25.1	0.0	1.087	0.716	0.137	63.8	0.235	1.68
6	9510	25.1	0.0	1.071	0.731	0.167	192.6	0.348	1.62
7	9516	25.1	0.0	1.080	0.712	0.135	84.4	0.358	1.68
8	9516	25.1	0.0	1.090	0.727	0.146	211.1	0.406	1.66
9	9642	25.0	0.0	1.094	0.775	0.193	212.7	0.513	1.56
10	9768	25.0	0.0	1.112	0.752	0.159	135.0	0.295	1.64
Mean	9581	25.1	0.0	1.090	0.739	0.158	167.4	0.391	1.63
Error	-	-	-	-	0.006	0.006	18.4	0.033	0.01

Table S13. GO-5-10-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})		A (m^2 g^{-1})		d_{pore} (nm)		ρ_{bulk} (g cm^{-3})
						aq	*g*	*aq*	*g*	*aq*	*g*	
1	11640	25.1	10.0	1.211	0.763	0.178	0.035	152.9	18.8	0.373	0.154	1.76
2	11694	25.1	9.8	1.230	0.782	0.190	0.048	222.8	76.4	0.432	0.142	1.74
3	11646	25.1	10.0	1.213	0.811	0.225	0.080	266.0	155.0	0.835	0.602	1.66
4	11460	25.1	10.2	1.189	0.723	0.162	0.014	53.6	0.4	0.309	0.116	1.82
5	11502	25.1	10.0	1.209	0.745	0.180	0.028	133.0	30.9	0.317	0.158	1.80
6	11526	25.1	10.2	1.192	0.735	0.182	0.024	76.6	14.0	0.339	0.132	1.80
7	11532	25.1	10.1	1.201	0.743	0.169	0.025	95.4	10.1	0.304	0.128	1.79
8	11532	25.1	10.0	1.211	0.749	0.171	0.026	172.4	27.8	0.415	0.320	1.79
9	11658	25.0	10.0	1.215	0.792	0.214	0.065	229.1	117.6	0.587	0.411	1.70
10	11784	25.0	9.8	1.234	0.777	0.184	0.042	161.2	49.4	0.292	0.243	1.76
Mean	11597	25.1	10.0	1.211	0.762	0.186	0.039	156.3	50.0	0.420	0.241	1.76
Error	-	-	-	-	0.009	0.006	0.006	20.8	15.3	0.051	0.048	0.02

Table S14. GO-5-10-w-s. *aq* and *g* refer to the porosity characterisation for aqueous and gaseous probe molecules, respectively.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.737	0.157	167.2	0.340	1.64
2	9678	25.1	0.0	1.109	0.747	0.148	222.4	0.438	1.64
3	9630	25.1	0.0	1.092	0.729	0.155	95.4	0.256	1.66
4	9444	25.1	0.0	1.068	0.719	0.159	160.6	0.286	1.65
5	9486	25.1	0.0	1.087	0.745	0.172	36.6	0.253	1.62
6	9510	25.1	0.0	1.071	0.715	0.144	102.7	0.257	1.66
7	9516	25.1	0.0	1.080	0.698	0.117	72.3	0.318	1.71
8	9516	25.1	0.0	1.090	0.721	0.138	91.3	0.314	1.67
9	9642	25.0	0.0	1.094	0.741	0.162	171.8	0.289	1.63
10	9768	25.0	0.0	1.112	0.778	0.185	197.8	0.362	1.58
Mean	9581	25.1	0.0	1.090	0.733	0.154	131.8	0.311	1.65
Error	-	-	-	-	0.007	0.006	18.1	0.017	0.01

Table S15. GO-5-15-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})		A (m^2 g^{-1})		d_{pore} (nm)		ρ_{bulk} (g cm^{-3})	E (GPa)
						aq	*g*	*aq*	*g*	*aq*	*g*		
1	12825	25.1	15.0	1.282	0.800	0.226	0.009	276.2	0.0	0.468	0.097	1.77	11.1
2	12879	25.1	14.8	1.301	0.811	0.217	0.014	265.9	0.0	0.437	0.117	1.78	23.2
3	12831	25.1	15.0	1.285	0.794	0.232	0.007	186.0	0.0	0.328	0.135	1.79	19.6
4	12645	25.1	15.2	1.261	0.787	0.239	0.011	185.3	0.0	0.324	0.123	1.77	8.3
5	12687	25.1	15.0	1.280	0.797	0.238	0.011	278.6	0.0	0.422	0.139	1.78	11.7
6	12711	25.1	15.2	1.263	0.792	0.238	0.011	258.9	0.0	0.393	0.102	1.77	23.1
7	12717	25.1	15.1	1.273	0.795	0.226	0.010	235.5	0.0	0.342	0.101	1.77	18.6
8	12717	25.1	15.0	1.282	0.798	0.233	0.008	227.8	0.0	0.345	0.095	1.78	13.2
9	12843	25.0	14.9	1.286	0.806	0.239	0.015	188.1	0.0	0.311	0.130	1.77	23.6
10	12969	25.0	14.7	1.305	0.834	0.249	0.029	257.4	45.4	0.394	0.142	1.73	28.9
Mean	12782	25.1	15.0	1.282	0.801	0.234	0.013	236.0	4.5	0.376	0.118	1.77	18.1
Error	-	-	-	-	0.004	0.003	0.002	11.3	4.5	0.016	0.005	0.00	2.0

Table S16. GO-5-15-w-s. *aq* and *g* refer to the porosity characterisation for aqueous and gaseous probe molecules, respectively.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.758	0.182	254.3	0.374	1.59
2	9678	25.1	0.0	1.109	0.802	0.201	309.8	0.462	1.53
3	9630	25.1	0.0	1.092	0.744	0.155	187.5	0.348	1.63
4	9444	25.1	0.0	1.068	0.742	0.260	287.0	0.478	1.59
5	9486	25.1	0.0	1.087	0.757	0.187	265.5	0.404	1.59
6	9510	25.1	0.0	1.071	0.734	0.173	153.3	0.360	1.62
7	9516	25.1	0.0	1.080	0.750	0.173	117.4	0.444	1.59
8	9516	25.1	0.0	1.090	0.713	0.259	458.9	0.888	1.69
9	9642	25.0	0.0	1.094	0.741	0.165	132.3	0.297	1.64
10	9768	25.0	0.0	1.112	0.785	0.194	213.2	0.513	1.57
Mean	9581	25.1	0.0	1.090	0.753	0.194	209.2	0.457	1.60
Error	-	-	-	-	0.008	0.011	31.9	0.050	0.01

Table S17. GO-5-20-d-s.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})		A (m^2 g^{-1})		d_{pore} (nm)		ρ_{bulk} (g cm^{-3})
						aq	*g*	*aq*	*g*	*aq*	*g*	
1	14160	25.1	20.0	1.362	0.866	0.301	0.005	393.5	0.0	0.548	0.119	1.74
2	14214	25.1	19.7	1.381	0.887	0.304	0.007	418.4	0.0	0.504	0.138	1.73
3	14166	25.1	20.0	1.365	0.869	0.305	0.006	381.1	0.0	0.388	0.128	1.74
4	13980	25.1	20.3	1.341	0.860	0.319	0.007	441.0	0.0	0.478	0.132	1.73
5	14022	25.1	20.0	1.360	0.870	0.317	0.006	453.2	0.0	0.546	0.100	1.73
6	14046	25.1	20.3	1.344	0.859	0.319	0.006	442.1	0.0	0.502	0.130	1.73
7	14052	25.1	20.1	1.353	0.864	0.314	0.006	330.6	0.2	0.431	0.113	1.73
8	14052	25.1	20.0	1.363	0.864	0.306	0.005	408.9	0.0	0.451	0.127	1.75
9	14178	25.0	19.9	1.366	0.867	0.312	0.005	375.6	0.0	0.355	0.113	1.75
10	14304	25.0	19.7	1.385	0.872	0.292	0.005	363.8	0.0	0.437	0.095	1.76
Mean	14117	25.1	20.0	1.362	0.868	0.309	0.006	400.8	0.0	0.464	0.120	1.74
Error	-	-	-	-	0.002	0.003	0.000	11.8	0.0	0.019	0.004	0.00

Table S18. GO-5-20-w-s. *aq* and *g* refer to the porosity characterisation for aqueous and gaseous probe molecules, respectively.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})	A (m^2 g^{-1})	d_{pore} (nm)	ρ_{bulk} (g cm^{-3})
1	9624	25.1	0.0	1.090	0.745	0.170	173.2	0.365	1.62
2	9678	25.1	0.0	1.109	0.791	0.196	272.7	0.566	1.55
3	9630	25.1	0.0	1.092	0.753	0.170	260.9	0.504	1.61
4	9444	25.1	0.0	1.068	0.733	0.170	215.4	0.350	1.61
5	9486	25.1	0.0	1.087	0.723	0.154	147.9	0.352	1.67
6	9510	25.1	0.0	1.071	0.728	0.165	128.3	0.329	1.63
7	9516	25.1	0.0	1.080	0.712	0.132	145.6	0.307	1.68
8	9516	25.1	0.0	1.090	0.750	0.163	150.5	0.395	1.61
9	9642	25.0	0.0	1.094	0.753	0.178	210.3	0.316	1.61
10	9768	25.0	0.0	1.112	0.800	0.207	301.2	0.497	1.54
Mean	9581	25.1	0.0	1.090	0.749	0.171	200.6	0.398	1.61
Error	-	-	-	-	0.009	0.006	18.3	0.027	0.01

Table S19. GO-5-10-d-l.

Model	N_{atm}	Oxygen content (%)	Water content (%)	m ($\times 10^5$ g mol^{-1})	d (nm)	v (cm^3 g^{-1})		A (m^2 g^{-1})		d_{pore} (nm)		ρ_{bulk} (g cm^{-3})
						aq	*g*	*aq*	*g*	*aq*	*g*	
1	11640	25.1	10.0	1.211	0.747	0.170	0.021	122.3	0.0	0.331	0.116	1.80
2	11694	25.1	9.8	1.230	0.794	0.210	0.061	216.4	89.1	0.338	0.333	1.72
3	11646	25.1	10.0	1.213	0.759	0.178	0.031	162.9	9.2	0.407	0.141	1.77
4	11460	25.1	10.2	1.189	0.747	0.190	0.036	146.1	48.6	0.348	0.129	1.76
5	11502	25.1	10.0	1.209	0.744	0.178	0.025	27.2	0.0	0.310	0.127	1.80
6	11526	25.1	10.2	1.192	0.747	0.189	0.033	158.2	30.6	0.292	0.144	1.77
7	11532	25.1	10.1	1.201	0.756	0.180	0.038	150.5	41.1	0.307	0.135	1.76
8	11532	25.1	10.0	1.211	0.772	0.193	0.049	222.5	86.5	0.325	0.140	1.74
9	11658	25.0	10.0	1.215	0.786	0.210	0.065	244.9	112.6	0.397	0.203	1.71
10	11784	25.0	9.8	1.234	0.811	0.218	0.074	268.9	117.1	0.495	0.218	1.68
Mean	11597	25.1	10.0	1.211	0.766	0.192	0.043	172.0	53.5	0.355	0.169	1.75
Error	-	-	-	-	0.007	0.005	0.005	21.0	13.5	0.018	0.020	0.01

Table S20. GO-5-10-w-l. *aq* and *g* refer to the porosity characterisation for aqueous and gaseous probe molecules, respectively.