Supporting Document for:

Molecular simulations of nitrogen-doped hierarchical carbon adsorbents for post-combustion CO_2 capture

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Table S1. Carbon dioxide capacity for SU-MAC-500 and SU-MAC-800 carbonaceous sorbents at 298K.

SU-MAC-500		SU-MAC-800	
Pressure (bar)	Adsorption (mmol/g)	Pressure (bar)	Adsorption mmol/g
4.80E-05	0.005530242	5.30E-04	0.001165907
8.12E-05	0.010010721	7.55E-04	0.002175467
1.08E-04	0.01362012	1.01E-03	0.003372644
1.28E-04	0.016242294	2.51E-03	0.010823729
3.06E-04	0.030858572	5.02E-03	0.023528098
5.40E-04	0.046314661	7.53E-03	0.036531761
8.20E-04	0.061958367	1.01E-02	0.048177432
1.06E-03	0.074086483	2.51E-02	0.113441437
2.65E-03	0.136076119	5.02E-02	0.211940499
5.13E-03	0.215523095	7.54E-02	0.308675065
7.53E-03	0.281845796	1.01E-01	0.402925936
1.01E-02	0.340681676	1.25E-01	0.4934736
2.70E-02	0.642602519	1.50E-01	0.582596266
5.03E-02	0.938689359	1.99E-01	0.745725007
7.60E-02	1.197686054	2.49E-01	0.905918878
1.02E-01	1.422741892	2.99E-01	1.065152327
1.25E-01	1.590319843	3.49E-01	1.221227553
1.49E-01	1.752863397	4.02E-01	1.400754936
2.00E-01	2.039185205	4.49E-01	1.542486375
2.51E-01	2.284758331	4.99E-01	1.689801662
3.01E-01	2.50087108	5.49E-01	1.838269454
3.52E-01	2.703886358	5.99E-01	1.983721969
4.02E-01	2.904283927	6.49E-01	2.128312338
4.49E-01	3.063137675	7.01E-01	2.277217904
4.99E-01	3.218449031	7.49E-01	2.415062986
5.49E-01	3.369235236	8.00E-01	2.556821228
6.00E-01	3.511668007	8.51E-01	2.700044671

6.50E-01	3.647820066	9.01E-01	2.841441079
7.00E-01	3.776293219	9.49E-01	2.974157956
7.51E-01	3.904051639	9.99E-01	3.109318324
8.00E-01	4.027454659		
8.50E-01	4.1452917		
9.00E-01	4.255780398		
9.50E-01	4.384834271		
1.00E+00	4.497449299		

Table S2. Pore size distributions for SU-MAC-500 and SU-MAC-800.

SU-MAC-500				SU-MAC-800			
N_2		CO_2		N_2		CO_2	
Pore size (nm)	dV/dD cc/nm/g	Pore size (nm)	dV/dD cc/nm/g	Pore size (nm)	dV/dD cc/nm/g	Pore size (nm)	dV/dD cc/nm/g
0.545	1.50E+00	0.3053	0	0.545	6.28E-01	0.3053	0.00E+00
0.571	1.96E+00	0.31934	0	0.571	9.12E-01	0.3193	1.54E-02
0.598	1.72E+00	0.33404	0	0.598	9.31E-01	0.334	1.17E-01
0.624	1.20E+00	0.34942	2.824	0.624	8.38E-01	0.3494	2.13E-02
0.651	5.84E-01	0.3655	2.40395	0.651	6.46E-01	0.3655	1.44E-01
0.677	1.61E-01	0.38232	0	0.677	5.26E-01	0.3823	1.51E-01
0.704	0.00E+00	0.39992	0	0.704	3.96E-01	0.3999	0.00E+00
0.744	0.00E+00	0.41832	0	0.744	2.09E-01	0.4183	0.00E+00
0.783	0.00E+00	0.43758	0	0.783	2.38E-01	0.4376	0.00E+00
0.823	1.37E-02	0.45772	0	0.823	3.73E-01	0.4577	5.38E-01
0.863	8.60E-02	0.4788	1.24865	0.863	5.48E-01	0.4788	2.18E-01
0.902	1.09E-01	0.50082	1.47825	0.902	6.86E-01	0.5008	1.20E+00
0.942	9.00E-02	0.52388	1.19005	0.942	7.09E-01	0.5239	1.57E-01
0.982	5.51E-02	0.548	0.919	0.982	6.43E-01	0.548	1.12E+00
1.022	1.90E-01	0.57322	0.7593	1.022	5.68E-01	0.5732	8.83E-01
1.061	9.25E-02	0.5996	0.6347	1.061	2.94E-01	0.5996	1.01E+00
1.114	6.04E-02	0.6272	0.50745	1.114	3.27E-01	0.6272	7.52E-01
1.167	4.19E-02	0.65606	0.383455	1.167	7.06E-01	0.6561	5.83E-01
1.22	3.25E-02	0.68626	0.270225	1.22	1.01E+00	0.6863	2.54E-01
1.273	0.00E+00	0.71786	0.1679	1.273	8.76E-01	0.7179	2.28E-01
1.326	0.00E+00	0.7509	0.147255	1.326	6.10E-01	0.7509	4.48E-01
1.379	0.00E+00	0.78546	0.35348	1.379	3.49E-01	0.7855	6.36E-01
1.432	0.00E+00	0.8216	0.41477	1.432	1.27E-01	0.8216	9.93E-01
1.498	0.00E+00	0.85942	0.26453	1.498	1.54E-01	0.8594	9.59E-01
1.564	0.00E+00	0.89898	0.21521	1.564	1.47E-01	0.899	6.92E-01
1.631	0.00E+00	0.94036	0.192275	1.631	1.01E-01	0.9404	5.77E-01
1.697	0.00E+00	0.98364	0.178525	1.697	1.45E-01	0.9836	5.10E-01

1.78	0.00E+00	1.02892	0.16912	1.78	8.92E-02	1.0289	4.63E-01
1.884	3.81E-02	1.07628	0.16231	1.884	3.03E-01	1.0763	4.39E-01
1.964	4.73E-02	1.12582	0.157215	1.964	3.99E-01	1.1258	4.02E-01
2.043	4.22E-02	1.17764	0.153245	2.043	3.60E-01	1.1776	3.96E-01
2.123	2.76E-02	1.23184	0.150095	2.123	3.36E-01	1.2318	3.87E-01
2.202	1.62E-02	1.28854	0.147675	2.202	3.00E-01	1.2885	3.68E-01
2.282	1.03E-02	1.34784	0.14567	2.282	2.79E-01	1.3478	3.53E-01
2.361	1.86E-02	1.40988	0.144115	2.361	3.33E-01	1.4099	3.55E-01
2.44	2.06E-02	1.47478	0.142835	2.44	2.59E-01	1.4748	3.55E-01
2.52	1.23E-02			2.52	2.57E-01		
2.599	1.02E-02			2.599	2.71E-01		
2.718	1.00E-02			2.718	1.62E-01		
2.838	1.06E-02			2.838	1.68E-01		
2.957	7.63E-03			2.957	1.50E-01		
3.076	9.87E-03			3.076	1.25E-01		
3.195	1.09E-02			3.195	1.38E-01		
3.314	1.29E-02			3.314	1.33E-01		
3.433	1.50E-02			3.433	1.84E-01		
3.553	1.89E-02			3.553	2.59E-01		
3.672	1.49E-02			3.672	1.88E-01		
3.791	1.38E-02			3.791	1.67E-01		
3.95	1.46E-02			3.95	1.36E-01		
4.109	1.41E-02			4.109	1.07E-01		
4.268	1.92E-02			4.268	8.82E-02		
4.427	1.88E-02			4.427	7.96E-02		
4.585	2.77E-02			4.585	9.43E-02		
4.744	4.67E-02			4.744	1.13E-01		
4.903	4.73E-02			4.903	1.11E-01		
5.102	5.25E-02			5.102	8.62E-02		
5.3	5.94E-02			5.3	8.37E-02		
5.499	4.44E-02			5.499	6.14E-02		
5.698	1.25E-02			5.698	1.45E-02		
5.896	6.07E-03			5.896	6.74E-03		
6.095	4.46E-03			6.095	4.78E-03		
6.333	2.45E-03			6.333	3.01E-03		
6.572	1.73E-03			6.572	2.75E-03		
6.81	1.31E-03			6.81	2.20E-03		
7.048	1.99E-03			7.048	1.78E-03		
7.326	3.06E-03			7.326	9.68E-04		
7.604	2.37E-03			7.604	6.73E-04		
7.882	2.11E-03			7.882	5.20E-04		
8.16	2.58E-03			8.16	2.18E-03		

8.478	2.42E-03	8.478	2.45E-03
8.796	2.93E-03	8.796	2.89E-03
9.114	2.51E-03	9.114	2.71E-03
9.432	1.87E-03	9.432	2.19E-03
9.789	1.61E-03	9.789	1.92E-03
10.147	1.54E-03	10.147	1.78E-03
10.504	1.57E-03	10.504	1.90E-03
10.901	1.26E-03	10.901	1.64E-03
11.298	1.02E-03	11.298	1.37E-03
11.696	9.47E-04	11.696	1.22E-03
12.133	9.80E-04	12.133	1.31E-03
12.57	9.14E-04	12.57	1.19E-03
13.006	7.08E-04	13.006	1.05E-03
13.483	9.78E-04	13.483	1.63E-03
13.96	7.82E-04	13.96	1.28E-03
14.476	6.82E-04	14.476	1.13E-03
14.993	7.86E-04	14.993	1.29E-03
15.549	6.46E-04	15.549	1.06E-03
16.105	5.42E-04	16.105	8.90E-04
16.701	6.83E-04	16.701	1.25E-03
17.296	7.25E-04	17.296	1.53E-03
17.932	5.15E-04	17.932	1.09E-03
18.568	5.15E-04	18.568	1.11E-03
19.243	4.22E-04	19.243	8.70E-04
19.918	3.95E-04	19.918	8.44E-04
20.633	3.69E-04	20.633	7.66E-04
21.388	3.04E-04	21.388	6.37E-04
22.143	2.86E-04	22.143	5.90E-04
22.937	3.43E-04	22.937	7.22E-04
23.771	3.06E-04	23.771	6.29E-04
24.645	2.77E-04	24.645	6.86E-04
25.519	3.07E-04	25.519	9.44E-04
26.433	2.83E-04	26.433	8.66E-04
27.386	2.61E-04	27.386	8.01E-04
28.379	2.37E-04	28.379	7.36E-04
29.412	2.50E-04	29.412	7.63E-04
30.484	2.00E-04	30.484	6.25E-04
31.557	1.61E-04	31.557	4.84E-04
32.669	1.80E-04	32.669	5.56E-04
33.821	1.60E-04	33.821	4.85E-04
35.012	1.58E-04	35.012	4.84E-04
36.244	1.35E-04	36.244	4.12E-04

37.515	1.38E-04	37.515	4.18E-04
38.826	1.19E-04	38.826	3.67E-04
40.176	1.55E-03	40.176	8.23E-03

Methods

Partitioning of the pore size distribution.

Pore volumes were estimated by integration of the differential pore volume over limits that center around the pore width of interest. For example, the 8 Å pore volume was estimated as:

$$\int_{7.5\ \text{Å}}^{8.5\ \text{Å}} \psi_x dx$$

where ψ_x is the differential pore volume taken from Table S2. More appropriately, this integral can be approximated as the sum of cumulative pore volumes over the same integral. For 8 Å, this becomes:

$$\sum_{i\,=\,7.5\ \text{Å}}^{i\,=\,8.5} \psi_i$$

Boundary definition for each pore is somewhat arbitrary, though an effort was made to ensure that the average of the upper and lower boundaries fell at or about the pore size of interest. Based on the PSDs provided in Table S2, the following boundaries were assumed:

Table S3. Boundaries for PSD partitioning.

Pore Size (Å)	Lower limit	Upper Limit
3.5	0	3.492
4	3.655	4.5772
5	4.788	5.0082
6	5.2388	6.272
7	6.5606	7.1786
8	7.509	8.216
9	8.5942	9.4036
10	9.8364	10.2892
12	10.7628	12.8854
14	13.4784	16.97
18	17.8	19.64
22	20.43	23.61
28	24.4	30.76
34	31.95	36.72
40	37.91	44.27
50	45.85	54.99
60	56.98	65.72
70	68.1	76.04

80	78.82	84.78
90	87.96	94.32
100	97.89	105.04
120	109.01	130.06
140	134.83	144.76
160	149.93	167.01
180	172.96	192.43
200	199.18	401.76

Differential volumes marked in blue font taken from NLDFT carbon model based on CO_2 adsorption at 273K; differential volumes marked in red taken from the QSDFT carbon model based on N_2 physisorption at 77K.

Here, the PSD is truncated at 200 Å and all volumes greater than 200 Å are treated as a 200 Å pore. This is reasonable as at this width, fluid-fluid interactions dominate and the pore density is assumed as the bulk fluid density.

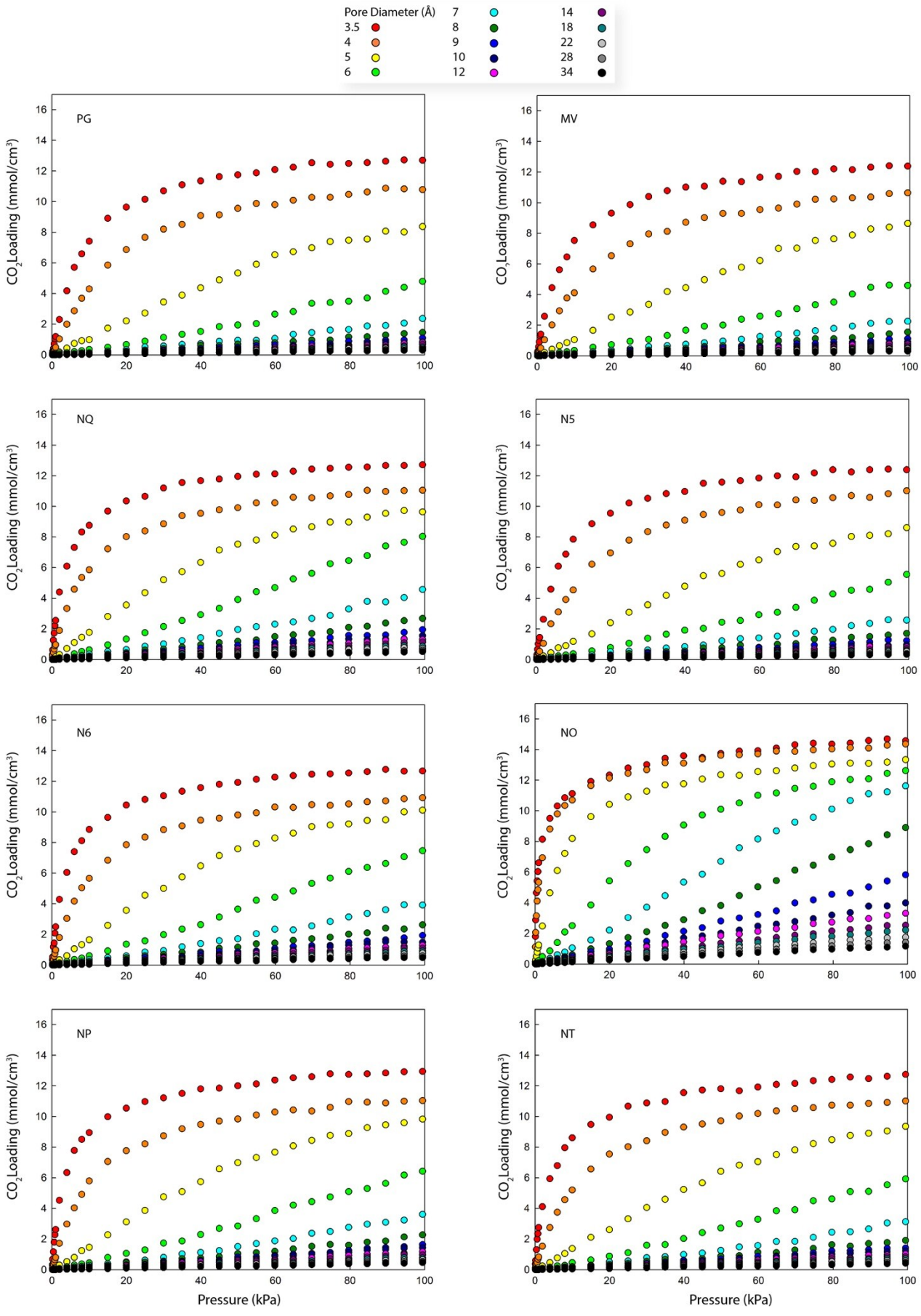
Pore Diameter (Å)
3.5
4
5
6
7
8
9
10
12
14
18
22
28
34
PG
MV
NQ
N5
N6
NO
NP
NT
CO2Loading (mmol/cm3)
Pressure (kPa)

Figure S1. Volume normalized pore densities for the 8 surfaces under study (3.5 – 34 Å).

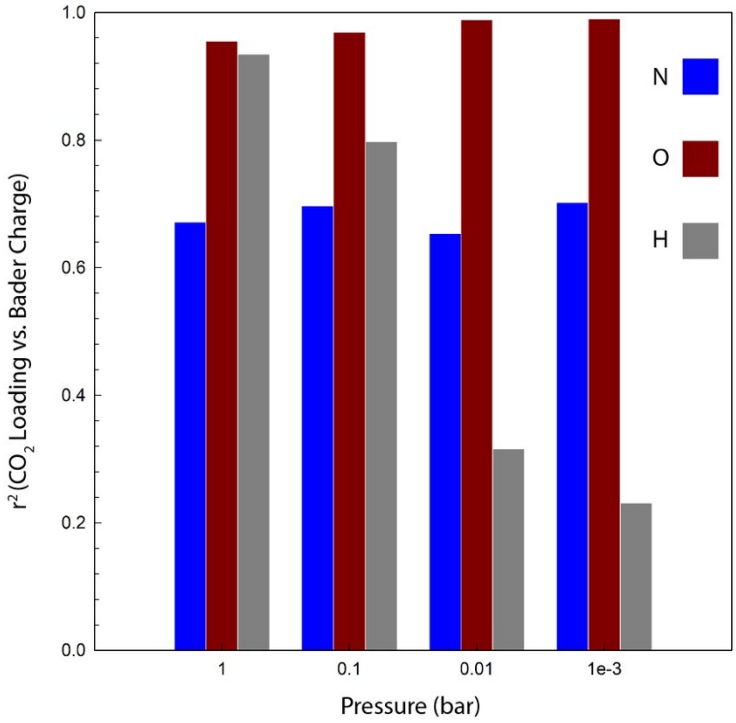

Figure S2. Correlation between Bader charge on select surface adatoms (N, O, and H) and CO_2 loading capacity, measured at 0.001, 0.01, 0.1, and 1 bar.

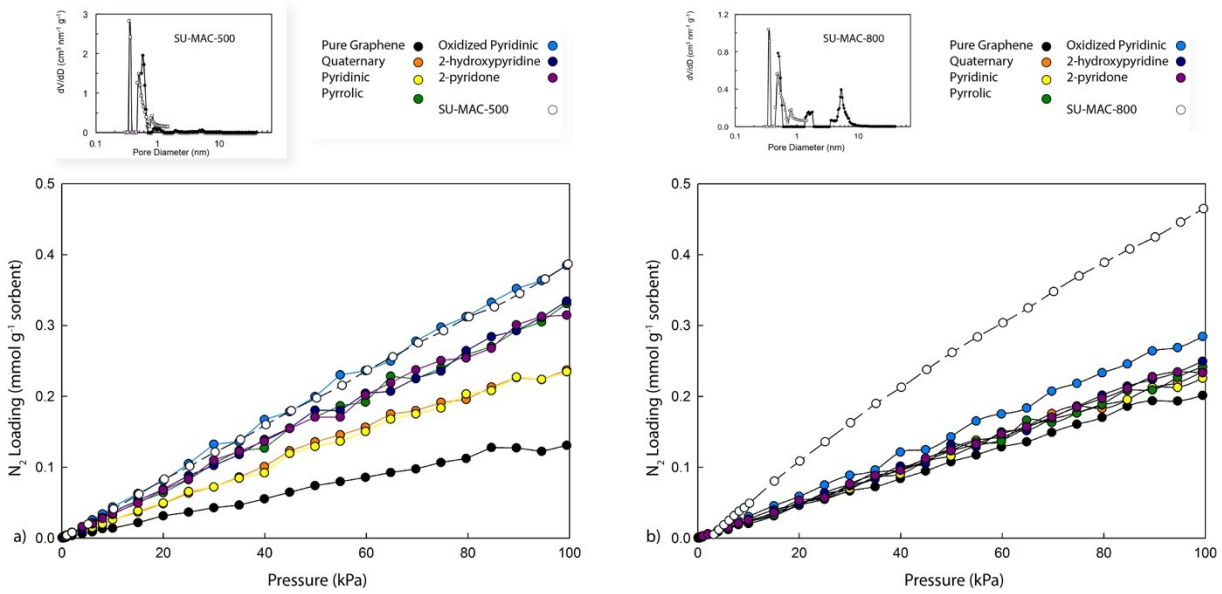

Figure S3. N_2 adsorption isotherms for the pure and *N*-modified surfaces. Isotherms are constructed as the weighted sum of individual slit-pore loading densities (excess), based on the pore-size distribution of a strong-performing hierarchical carbonaceous sorbent (inset).

Method: Ideal Adsorbed Solution Theory (IAST) Selectivity

The IAST method can be used to predict the equilibrium adsorption of each component in a gas mixture from the pure (ideal) adsorption isotherms of each component. Typically, IAST predictions more accurately describe adsorption at working conditions as this method is not as vulnerable to surface energy heterogeneity as the Henry's Law method. Because this study deals with surface nitrogen substitution, a condition that necessarily introduces surface heterogeneity, the IAST method is chosen to calculate CO_2/N_2 selectivity. Further, we assume that our gas-gas solution behaves ideally, and that the entire surface is equally accessible to all components. For more on IAST theory, readers are referred to the original work of Myers and Prausnitz(1), or the text *Principles of adorption and adsorption processes,* (1984) (2). IAST selectivity calculations were calculated by the python code *pyIAST*, developed by Simon et al. (3). Readers are directed to the methodology outlined in the *pyIAST* user manual, accessible at: http://corymsimon.com/portfolio_page/pyiast-ideal-adsorbed-solution-theory-iast-python-package/.

VASP-optimized models: coordinates and Bader charges

PURE GRAPHENE-PG

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	0	8.544	0.0002	C	0
2	0	4.272	0.0002	C	0
3	4.9329	8.544	0.0002	C	0
4	4.9329	4.272	0.0002	C	0
5	1.2332	0.712	0.0001	C	0
6	1.2332	4.984	0.0001	C	0
7	6.1661	0.712	0.0001	C	0
8	6.1661	4.984	0.0001	C	0
9	1.2332	2.136	0.0002	C	0
10	1.2332	6.408	0.0002	C	0
11	6.1661	2.136	0.0002	C	0
12	6.1661	6.408	0.0002	C	0
13	0	2.848	0.0001	C	0
14	0	7.12	0.0001	C	0
15	4.9329	2.848	0.0001	C	0
16	4.9329	7.12	0.0001	C	0
17	2.4664	8.544	0.0002	C	0
18	2.4664	4.272	0.0002	C	0
19	7.3993	8.544	0.0002	C	0
20	7.3993	4.272	0.0002	C	0
21	3.6997	0.712	0.0001	C	0
22	3.6997	4.984	0.0001	C	0
23	8.6325	0.712	0.0001	C	0
24	8.6325	4.984	0.0001	C	0
25	3.6997	2.136	0.0002	C	0
26	3.6997	6.408	0.0002	C	0
27	8.6325	2.136	0.0002	C	0

28	8.6325	6.408	0.0002	C	0
29	2.4664	2.848	0.0001	C	0
30	2.4664	7.12	0.0001	C	0
31	7.3993	2.848	0.0001	C	0
32	7.3993	7.12	0.0001	C	0
33	0	0	3.35	C	0
34	0	4.272	3.35	C	0
35	4.9329	0	3.35	C	0
36	4.9329	4.272	3.35	C	0
37	0	1.424	3.35	C	0
38	0	5.696	3.35	C	0
39	4.9329	1.424	3.35	C	0
40	4.9329	5.696	3.35	C	0
41	1.2332	2.136	3.35	C	0
42	1.2332	6.408	3.35	C	0
43	6.1661	2.136	3.35	C	0
44	6.1661	6.408	3.35	C	0
45	1.2332	3.56	3.35	C	0
46	1.2332	7.832	3.35	C	0
47	6.1661	3.56	3.35	C	0
48	6.1661	7.832	3.35	C	0
49	2.4664	0	3.35	C	0
50	2.4664	4.272	3.35	C	0
51	7.3993	0	3.35	C	0
52	7.3993	4.272	3.35	C	0
53	2.4664	1.424	3.35	C	0
54	2.4664	5.696	3.35	C	0
55	7.3993	1.424	3.35	C	0
56	7.3993	5.696	3.35	C	0
57	3.6997	2.136	3.35	C	0
58	3.6997	6.408	3.35	C	0
59	8.6325	2.136	3.35	C	0
60	8.6325	6.408	3.35	C	0
61	3.6997	3.56	3.35	C	0
62	3.6997	7.832	3.35	C	0
63	8.6325	3.56	3.35	C	0
64	8.6325	7.832	3.35	C	0
65	0	0	6.7103	C	0
66	0	4.272	6.7103	C	0
67	4.9329	0	6.7103	C	0
68	4.9329	4.272	6.7103	C	0
69	1.2332	0.7123	6.7119	C	0
70	1.2332	4.9843	6.7119	C	0
71	6.1661	0.7123	6.7119	C	0
72	6.1661	4.9843	6.7119	C	0
73	1.2332	2.136	6.7103	C	0
74	1.2332	6.408	6.7103	C	0
75	6.1661	2.136	6.7103	C	0
76	6.1661	6.408	6.7103	C	0
77	0	2.8483	6.7119	C	0
78	0	7.1203	6.7119	C	0
79	4.9329	2.8483	6.7119	C	0
80	4.9329	7.1203	6.7119	C	0
81	2.4664	0	6.7103	C	0
82	2.4664	4.272	6.7103	C	0
83	7.3993	0	6.7103	C	0
84	7.3993	4.272	6.7103	C	0
85	3.6997	0.7123	6.7119	C	0
86	3.6997	4.9843	6.7119	C	0
87	8.6325	0.7123	6.7119	C	0
88	8.6325	4.9843	6.7119	C	0
89	3.6997	2.136	6.7103	C	0
90	3.6997	6.408	6.7103	C	0
91	8.6325	2.136	6.7103	C	0
92	8.6325	6.408	6.7103	C	0
93	2.4664	2.8483	6.7119	C	0
94	2.4664	7.1203	6.7119	C	0
95	7.3993	2.8483	6.7119	C	0
96	7.3993	7.1203	6.7119	C	0

MONO-VACANCY GRAPHENE-MV

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	4.9329	8.542	0.0167	C	-0.019
2	0	8.542	0.0168	C	-0.019
3	0	4.27	0.0168	C	-0.019
4	4.9329	4.27	0.0165	C	-0.0189
5	6.1661	4.982	0.0158	C	0.0354
6	6.1661	0.71	0.0158	C	0.0353
7	1.2332	0.71	0.0159	C	0.0353
8	1.2332	4.982	0.0159	C	0.0353
9	6.1662	2.1341	0.016	C	-0.0435
10	1.2333	2.1341	0.0161	C	-0.0436

11	1.2333	6.4061	0.0161	C	-0.0436
12	6.1662	6.4061	0.016	C	-0.0436
13	0	7.118	0.0163	C	0.0595
14	4.9329	2.846	0.016	C	0.0597
15	4.9329	7.118	0.0161	C	0.0597
16	0	2.846	0.0163	C	0.0595
17	2.4665	8.542	0.0168	C	-0.05
18	2.4664	4.2701	0.0168	C	-0.05
19	7.3993	8.542	0.0168	C	-0.05
20	7.3993	4.2701	0.0168	C	-0.05
21	3.6996	4.982	0.0158	C	0.0354
22	8.6325	4.982	0.0159	C	0.0353
23	3.6996	0.71	0.0158	C	0.0353
24	8.6325	0.71	0.0159	C	0.0353
25	8.6325	2.1341	0.0161	C	-0.0436
26	3.6996	2.1341	0.016	C	-0.0435
27	8.6325	6.4061	0.0161	C	-0.0436
28	3.6996	6.4061	0.016	C	-0.0436
29	2.4664	7.1183	0.0158	C	0.0297
30	7.3993	2.8463	0.0157	C	0.0296
31	2.4664	2.8463	0.0157	C	0.0296
32	7.3993	7.1183	0.0158	C	0.0297
33	0	4.2725	3.3512	C	-0.0238
34	4.9329	4.2728	3.354	C	-0.0198
35	0	0.0006	3.3511	C	-0.0229
36	4.9329	0.0011	3.3508	C	-0.0207
37	0	1.4246	3.3508	C	0.0618
38	0	5.6966	3.3513	C	0.0613
39	4.9329	5.6967	3.3516	C	0.0658
40	4.9329	1.425	3.3516	C	0.0617
41	1.2334	2.1364	3.3498	C	-0.0477
42	1.2336	6.4085	3.3508	C	-0.0485
43	6.1663	2.137	3.3505	C	-0.0451
44	6.1661	6.4087	3.3503	C	-0.0468
45	6.1661	3.5607	3.3515	C	0.0395
46	6.1661	7.8327	3.3506	C	0.037
47	1.2333	3.5604	3.3506	C	0.0384
48	1.2333	7.8326	3.351	C	0.0375
49	7.3991	0.0006	3.3509	C	-0.0518
50	7.3991	4.2723	3.3512	C	-0.0514
51	2.4666	0.0006	3.3509	C	-0.0518
52	2.4666	4.2723	3.3512	C	-0.0514
53	7.3993	1.4246	3.3503	C	0.0334
54	2.4665	1.4246	3.3503	C	0.0334
55	2.4666	5.6964	3.3512	C	0.0351
56	7.3991	5.6964	3.3512	C	0.0351
57	8.6324	2.1364	3.3498	C	-0.0477
58	8.6322	6.4085	3.3508	C	-0.0485
59	3.6994	2.137	3.3505	C	-0.0451
60	3.6997	6.4087	3.3503	C	-0.0468
61	3.6996	3.5607	3.3515	C	0.0395
62	8.6324	3.5604	3.3506	C	0.0384
63	3.6997	7.8327	3.3506	C	0.037
64	8.6325	7.8326	3.351	C	0.0375
65	4.9329	0.0112	6.6925	C	0.0386
66	0	4.2645	6.6935	C	0.0009
67	0	8.5362	6.6931	C	-0.0143
68	6.2156	4.9882	6.6982	C	-0.1475
69	1.2358	0.6999	6.6921	C	0.0198
70	1.2322	4.9866	6.6948	C	-0.0325
71	6.1553	0.7362	6.6931	C	0.0342
72	6.1572	2.1882	6.6934	C	-0.0122
73	1.2322	2.1278	6.6913	C	0.0056
74	1.2396	6.4071	6.6948	C	0.0409
75	6.1389	6.382	6.6946	C	0.0263
76	4.9329	7.1307	6.692	C	0.0408
77	4.9329	2.8705	6.6909	C	-0.1027
78	0	7.1174	6.6945	C	0.0619
79	0	2.8413	6.6916	C	-0.0059
80	7.3868	0.0056	6.6932	C	0.0382
81	7.388	4.2585	6.6957	C	0.0301
82	2.4789	0.0056	6.6932	C	0.0382
83	2.4777	4.2585	6.6957	C	0.0301
84	3.6501	4.9882	6.6982	C	-0.1575
85	8.6299	0.6999	6.6921	C	0.0198
86	3.7105	0.7362	6.6931	C	0.0342
87	8.6336	4.9866	6.6948	C	-0.0325
88	8.6336	2.1278	6.6913	C	0.0056
89	8.6261	6.4071	6.6948	C	0.0409
90	3.7086	2.1882	6.6934	C	-0.0122
91	3.7269	6.382	6.6946	C	0.0263
92	7.4173	2.8386	6.6927	C	0.0086
93	7.3899	7.1138	6.6946	C	-0.0351
94	2.4485	2.8386	6.6927	C	0.0086

95	2.4758	7.1138	6.6946	C	-0.0351

PYRIDINIC NITROGEN-N6

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	2.4603	7.0533	0.0343	C	0.0045
2	7.3933	7.0534	0.0344	C	0.0041
3	7.3932	2.7814	0.0345	C	0.0042
4	2.4603	2.7813	0.0343	C	0.0044
5	3.6934	3.4934	0.0338	C	-0.0155
6	3.6935	7.7654	0.0336	C	-0.0158
7	8.6264	7.7654	0.0337	C	-0.0157
8	8.6264	3.4934	0.0337	C	-0.0157
9	3.6934	0.6454	0.0339	C	0.004
10	8.6262	0.6453	0.034	C	0.004
11	8.6262	4.9173	0.034	C	0.004
12	3.6933	4.9174	0.0341	C	0.0042
13	7.3932	5.6294	0.0336	C	-0.0119
14	2.4603	1.3574	0.0333	C	-0.0116
15	2.4603	5.6295	0.0335	C	-0.0118
16	7.3932	1.3574	0.0335	C	-0.0118
17	9.8597	7.0533	0.0333	C	0.0077
18	9.8597	2.7813	0.0333	C	0.0078
19	4.9269	7.0533	0.0334	C	0.0077
20	4.9268	2.7813	0.0335	C	0.0078
21	1.2273	3.4932	0.033	C	0.0091
22	6.1601	3.4933	0.0332	C	0.0087
23	1.2273	7.7653	0.0329	C	0.009
24	6.1602	7.7653	0.0331	C	0.009
25	6.1602	0.6453	0.0333	C	0.0277
26	1.2272	0.6453	0.0331	C	0.0276
27	6.1602	4.9173	0.0335	C	0.0278
28	1.2272	4.9173	0.0332	C	0.0277
29	9.8597	5.6291	0.0327	C	-0.0148
30	4.9267	1.3571	0.0328	C	-0.0147
31	9.8597	1.3571	0.0327	C	-0.0146
32	4.9267	5.6292	0.0329	C	-0.0148
33	7.392	2.7843	3.3509	C	-0.0128
34	2.459	2.7848	3.3562	C	-0.003
35	7.3918	7.0565	3.3497	C	-0.0124
36	2.4588	7.0571	3.3504	C	-0.0101
37	7.3921	8.4807	3.3494	C	0.0191
38	7.3921	4.2085	3.351	C	0.0196
39	2.4593	4.2082	3.3532	C	0.0264
40	2.4593	8.4808	3.3509	C	0.0212
41	8.6252	0.6485	3.3491	C	-0.0108
42	8.6255	4.9204	3.3503	C	-0.0114
43	3.6923	0.6491	3.3514	C	-0.007
44	3.692	4.9204	3.3529	C	-0.0095
45	3.692	2.0729	3.3535	C	0.0058
46	3.692	6.3447	3.3513	C	0.0032
47	8.6252	2.0724	3.3501	C	0.0032
48	8.625	6.3444	3.3495	C	0.0035
49	4.9249	7.0568	3.3505	C	-0.0116
50	4.9249	2.7844	3.3532	C	-0.0105
51	9.8583	7.0567	3.3497	C	-0.011
52	9.8585	2.7843	3.3517	C	-0.0092
53	4.9253	8.481	3.3502	C	0.0026
54	9.8587	8.4809	3.3497	C	0.003
55	9.859	4.2086	3.3513	C	0.0063
56	4.9252	4.2087	3.3535	C	0.0038
57	6.1588	0.6486	3.3497	C	-0.0084
58	6.1589	4.9205	3.3517	C	-0.0099
59	1.2259	0.6491	3.3512	C	-0.0054
60	1.2262	4.9205	3.3513	C	-0.008
61	1.226	2.0729	3.3525	C	0.0266
62	6.1585	2.0726	3.3508	C	0.0244
63	1.2259	6.3446	3.3499	C	0.0249
64	6.1586	6.3447	3.3504	C	0.0241
65	2.4582	7.0405	6.6776	C	0.0234
66	7.4115	2.7833	6.6769	C	0.0275
67	7.3878	7.0554	6.677	C	0.0099
68	8.6291	7.7123	6.6754	C	0.0125
69	8.6582	3.4671	6.679	C	-0.0311
70	3.6307	7.8736	6.6783	C	-0.0068
71	3.5539	0.8346	6.6774	C	0.0074
72	8.5713	0.5995	6.6742	C	0.0002
73	8.6761	4.8897	6.6787	C	0.0167
74	3.7948	4.9292	6.6691	C	0.6002
75	2.5096	5.5768	6.6739	C	-0.0337
76	2.2298	1.5666	6.6787	C	-0.002
77	7.438	5.6384	6.6781	C	-0.0323
78	7.3513	1.3619	6.6739	C	0.0022

79	4.8995	7.1456	6.6785	C	-0.0148
80	4.9489	2.8908	6.668	C	0.5442
81	0.0205	6.9821	6.6757	C	-0.015
82	9.8639	2.7039	6.6779	C	0.0428
83	1.3278	3.1814	6.6786	C	0.0156
84	6.1384	7.8115	6.6771	C	0.0107
85	1.2214	7.7457	6.677	C	0.0317
86	6.204	3.5414	6.6764	C	-0.0033
87	6.0928	0.6979	6.6739	C	-0.0248
88	6.1991	4.965	6.6769	C	0.0011
89	1.1617	0.6417	6.6777	C	-0.0267
90	1.3516	4.7176	6.6773	C	-0.0099
91	4.8587	1.4476	6.6719	C	0.0238
92	4.9714	5.7061	6.6771	C	0.0022
93	9.7693	1.2918	6.6759	C	-0.0302
94	0.0804	5.5194	6.678	C	0.0104
95	3.8171	3.5954	6.6567	N	-1.2612

PYROLLIC NITROGEN-N5

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	0.0003	8.5427	0.0129	C	-0.0212
2	0.0003	4.2707	0.0129	C	-0.0213
3	4.9331	8.5427	0.013	C	-0.0213
4	4.9331	4.2707	0.0127	C	-0.021
5	1.2336	0.7107	0.012	C	0.0369
6	1.2336	4.9827	0.0118	C	0.037
7	6.1665	0.7107	0.0119	C	0.0369
8	6.1664	4.9827	0.0118	C	0.0369
9	1.2336	2.1347	0.0121	C	-0.0464
10	1.2336	6.4067	0.012	C	-0.0466
11	6.1665	2.1347	0.012	C	-0.0464
12	6.1665	6.4067	0.012	C	-0.0465
13	0.0003	2.8466	0.0122	C	0.063
14	0.0003	7.1186	0.0121	C	0.063
15	4.9332	2.8466	0.0121	C	0.0629
16	4.9332	7.1186	0.0121	C	0.0631
17	2.4667	8.5427	0.0127	C	-0.05
18	2.4667	4.2707	0.0125	C	-0.0501
19	7.3996	8.5427	0.0127	C	-0.0501
20	7.3996	4.2707	0.0126	C	-0.0501
21	3.6999	0.7107	0.0119	C	0.0362
22	3.6999	4.9827	0.0116	C	0.0359
23	8.6327	0.7107	0.0118	C	0.0361
24	8.6327	4.9827	0.0118	C	0.0361
25	3.6998	2.1347	0.012	C	-0.0465
26	3.6998	6.4067	0.0118	C	-0.0469
27	8.6327	2.1347	0.012	C	-0.0468
28	8.6327	6.4067	0.012	C	-0.0468
29	2.4667	2.8469	0.0118	C	0.0323
30	2.4667	7.1188	0.0118	C	0.0324
31	7.3996	2.8468	0.0118	C	0.0323
32	7.3996	7.1189	0.0119	C	0.0323
33	9.8656	0.0006	3.3525	C	-0.0223
34	0.0001	4.2728	3.3518	C	-0.0215
35	4.9328	0.0009	3.3552	C	-0.02
36	4.9329	4.2729	3.3521	C	-0.0199
37	0	1.4247	3.3524	C	0.0627
38	0	5.6969	3.3509	C	0.0622
39	4.933	1.425	3.355	C	0.064
40	4.9328	5.6968	3.3515	C	0.0621
41	1.2334	2.1368	3.3526	C	-0.0458
42	1.2333	6.4088	3.3499	C	-0.0461
43	6.1662	2.1368	3.3521	C	-0.0459
44	6.1662	6.4088	3.3515	C	-0.0461
45	1.2334	3.5609	3.3514	C	0.0387
46	1.2331	7.8328	3.3512	C	0.0386
47	6.166	3.5608	3.3515	C	0.039
48	6.166	7.8327	3.3523	C	0.0395
49	2.4662	0.0008	3.3534	C	-0.0503
50	2.4664	4.2729	3.3513	C	-0.0502
51	7.3991	0.0005	3.3526	C	-0.0514
52	7.3992	4.2727	3.3515	C	-0.0508
53	2.4664	1.4248	3.3538	C	0.0355
54	2.4663	5.6968	3.3497	C	0.0353
55	7.3992	1.4246	3.352	C	0.0334
56	7.3992	5.6966	3.3511	C	0.034
57	3.6996	2.1371	3.355	C	-0.0443
58	3.6993	6.4091	3.3503	C	-0.0454
59	8.6324	2.1367	3.352	C	-0.047
60	8.6323	6.4087	3.3514	C	-0.0466
61	3.6996	3.5608	3.353	C	0.0391
62	3.6994	7.8327	3.3525	C	0.0395

63	8.6325	3.5607	3.3516	C	0.0381
64	8.6323	7.8326	3.3521	C	0.0389
65	9.8119	8.5122	6.6952	C	0.0087
66	0.0232	4.2966	6.6977	C	-0.0154
67	5.0649	8.4618	6.6859	C	-0.1477
68	4.9689	4.2999	6.6966	C	0.026
69	1.1043	0.7198	6.6948	C	-0.0352
70	1.3003	4.9552	6.6989	C	-0.0277
71	6.1723	0.6832	6.6933	C	-0.0732
72	6.2124	4.9932	6.6991	C	-0.0476
73	1.1037	2.131	6.6959	C	0.0416
74	1.3003	6.4391	6.6977	C	0.0219
75	6.1718	2.166	6.6951	C	0.0066
76	6.2119	6.3994	6.6973	C	0.0435
77	9.8124	2.8811	6.6984	C	0.015
78	0.0227	7.0971	6.6961	C	0.0011
79	5.0641	2.9304	6.6892	C	-0.1476
80	4.9693	7.0927	6.694	C	0.0294
81	2.3947	0.2134	6.6975	C	0.3091
82	2.5193	4.1527	6.6992	C	0.0107
83	7.4125	8.5364	6.6982	C	0.0151
84	7.4288	4.2748	6.6995	C	0.014
85	3.702	4.9727	6.699	C	-0.0211
86	8.6135	0.7078	6.6981	C	-0.0571
87	8.6589	4.9923	6.6979	C	-0.0391
88	3.7012	6.4205	6.6979	C	0.0601
89	8.6131	2.1413	6.6996	C	0.0304
90	8.6587	6.4008	6.6961	C	0.0615
91	2.3949	2.6377	6.6989	C	0.3095
92	2.5194	7.2418	6.699	C	0.0129
93	7.4123	2.8566	6.7008	C	0.0162
94	7.4291	7.118	6.6972	C	0.0161
95	4.2082	1.4206	6.7009	H	0.4579
96	3.1675	1.425	6.7028	N	-0.9579

QUATERNARY NITROGEN-NQ

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	4.9329	8.5429	0.017	C	-0.0223
2	9.8657	8.5429	0.0168	C	-0.0218
3	9.8658	4.2709	0.0169	C	-0.0222
4	4.9329	4.2709	0.0171	C	-0.0223
5	1.2332	4.9829	0.0162	C	0.0347
6	6.1661	0.7109	0.016	C	0.0347
7	1.2332	0.7109	0.016	C	0.0344
8	6.1661	4.9829	0.0162	C	0.0348
9	1.2332	2.1349	0.0161	C	-0.048
10	1.2332	6.4069	0.0162	C	-0.048
11	6.1661	2.1349	0.0161	C	-0.0479
12	6.1661	6.4069	0.0162	C	-0.0478
13	9.8657	2.8469	0.0161	C	0.0598
14	9.8658	7.1189	0.0161	C	0.0598
15	4.9329	2.847	0.0162	C	0.0598
16	4.9329	7.1189	0.0163	C	0.0597
17	2.4664	4.2709	0.0171	C	-0.0523
18	7.3993	8.5429	0.0168	C	-0.0522
19	7.3993	4.2709	0.0169	C	-0.0522
20	2.4664	8.5429	0.017	C	-0.0522
21	8.6325	4.9829	0.0161	C	0.0347
22	3.6997	0.7109	0.0163	C	0.0346
23	3.6997	4.9829	0.0162	C	0.0347
24	8.6325	0.7109	0.0159	C	0.0345
25	3.6997	2.1349	0.0163	C	-0.048
26	3.6997	6.4069	0.0163	C	-0.048
27	8.6325	2.1349	0.016	C	-0.0479
28	8.6325	6.4069	0.0162	C	-0.0479
29	7.3993	2.8469	0.0161	C	0.0311
30	2.4664	2.847	0.0162	C	0.0312
31	7.3993	7.1189	0.0161	C	0.0312
32	2.4664	7.1189	0.0163	C	0.0312
33	4.9331	4.2731	3.3532	C	-0.0234
34	9.8656	0.0009	3.3523	C	-0.0231
35	9.8656	4.273	3.353	C	-0.0227
36	4.9332	0.0009	3.3534	C	-0.0274
37	9.8656	5.697	3.3531	C	0.0607
38	4.9332	1.4252	3.353	C	0.0546
39	9.8656	1.4249	3.3516	C	0.0598
40	4.9331	5.697	3.3531	C	0.0595
41	1.233	6.4088	3.3526	C	-0.0499
42	6.1665	2.1372	3.3517	C	-0.0488
43	6.1663	6.4088	3.3526	C	-0.0496
44	1.2328	2.1372	3.3517	C	-0.0492
45	6.1665	7.8328	3.3529	C	0.0339

46	1.233	3.5611	3.3528	C	0.0329
47	1.2328	7.8328	3.3529	C	0.034
48	6.1663	3.5611	3.3528	C	0.0337
49	2.4661	0.0009	3.3534	C	-0.0566
50	2.4663	4.2731	3.3532	C	-0.0522
51	7.3995	0.0009	3.3523	C	-0.0526
52	7.3995	4.273	3.353	C	-0.0518
53	7.3995	1.4249	3.3516	C	0.0308
54	7.3995	5.697	3.3531	C	0.0311
55	2.4661	1.4252	3.353	C	0.0259
56	2.4662	5.697	3.3531	C	0.0301
57	8.6325	2.137	3.3512	C	-0.0478
58	8.6325	6.409	3.3525	C	-0.0482
59	3.6997	6.4086	3.3527	C	-0.0515
60	3.6997	2.1374	3.3527	C	-0.0517
61	3.6997	7.8327	3.3535	C	0.0312
62	8.6325	7.8328	3.3524	C	0.0343
63	8.6325	3.561	3.3525	C	0.0343
64	3.6997	3.5614	3.3531	C	0.0317
65	4.9282	4.2652	6.6903	C	-0.0115
66	0.0066	8.5428	6.6953	C	-0.0155
67	4.9237	0.0058	6.691	C	0.3266
68	0.0036	4.2748	6.6911	C	0.0409
69	1.2434	0.7149	6.6945	C	-0.02
70	6.156	0.7149	6.6945	C	-0.0091
71	6.1693	2.1371	6.6927	C	0.0309
72	1.23	2.1371	6.6927	C	0.0351
73	1.2367	6.415	6.691	C	0.0337
74	6.1626	6.415	6.691	C	0.0164
75	4.9235	7.1306	6.6922	C	0.0253
76	4.9297	2.8371	6.6913	C	0.0375
77	0.003	7.1207	6.6934	C	0.0667
78	0.0028	2.8465	6.6941	C	-0.0184
79	2.4712	4.2652	6.6903	C	-0.0137
80	7.3957	4.2748	6.6911	C	0.0374
81	2.4756	0.0058	6.691	C	0.3348
82	7.3927	8.5428	6.6953	C	-0.0353
83	8.6325	4.9862	6.6915	C	-0.0199
84	3.6997	4.9847	6.691	C	0.0359
85	8.6325	0.7126	6.697	C	0.0444
86	3.6997	6.4048	6.6908	C	-0.0178
87	8.6325	6.4078	6.6918	C	0.0401
88	3.6997	2.1228	6.6891	C	0.3731
89	8.6325	2.1326	6.6952	C	-0.044
90	7.3965	2.8465	6.6941	C	-0.0209
91	2.4696	2.8371	6.6913	C	0.0544
92	2.4758	7.1306	6.6922	C	0.0348
93	7.3963	7.1207	6.6934	C	0.064
94	6.1621	4.9843	6.6907	C	-0.0386
95	1.2373	4.9843	6.6907	C	-0.0654
96	3.6997	0.7148	6.6903	N	-1.1737

OXIDIZED PYRIDINIC-NO

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	9.8657	8.5422	0.0538	C	-0.0189
2	9.8657	4.2702	0.0547	C	-0.0181
3	4.9328	8.5421	0.0533	C	-0.0189
4	4.9328	4.2702	0.054	C	-0.0186
5	1.2333	0.7101	0.0538	C	0.0362
6	6.1661	0.7101	0.0537	C	0.0361
7	6.1661	4.9821	0.0535	C	0.0357
8	1.2333	4.9821	0.0542	C	0.0357
9	1.2332	6.4061	0.0541	C	-0.0431
10	6.1661	2.1341	0.0546	C	-0.0437
11	1.2332	2.1341	0.0547	C	-0.0427
12	6.1661	6.4061	0.0533	C	-0.0436
13	4.9328	2.8461	0.0538	C	0.06
14	4.9328	7.118	0.0523	C	0.0609
15	9.8657	2.8461	0.054	C	0.0597
16	9.8657	7.1181	0.0532	C	0.0598
17	7.3992	4.27	0.0547	C	-0.049
18	2.4664	8.542	0.054	C	-0.0494
19	2.4664	4.2701	0.0548	C	-0.049
20	7.3993	8.542	0.054	C	-0.0493
21	8.6324	4.9821	0.0542	C	0.0357
22	3.6995	4.9821	0.0536	C	0.0358
23	8.6324	0.7101	0.0538	C	0.036
24	3.6995	0.7101	0.0536	C	0.0361
25	8.6325	6.4061	0.054	C	-0.0431
26	8.6325	2.1341	0.0546	C	-0.0428
27	3.6995	6.4061	0.0533	C	-0.0431
28	3.6996	2.1341	0.0546	C	-0.0438

29	2.4664	2.8462	0.0543	C	0.03
30	7.3992	2.8462	0.0543	C	0.03
31	2.4664	7.1182	0.0531	C	0.03
32	7.3993	7.1182	0.0531	C	0.0302
33	4.9329	4.2756	3.349	C	-0.0116
34	0	4.275	3.3489	C	-0.017
35	4.9329	0.0033	3.3401	C	-0.0184
36	0	0.0026	3.3413	C	-0.0204
37	0	1.4268	3.3487	C	0.0583
38	4.9329	1.4271	3.3527	C	0.007
39	4.9329	5.6993	3.3355	C	0.0608
40	9.8657	5.6989	3.3417	C	0.0588
41	6.1659	6.4109	3.3327	C	-0.0421
42	1.2333	2.1388	3.3514	C	-0.0436
43	1.2336	6.4105	3.3376	C	-0.0437
44	6.1666	2.1395	3.355	C	-0.0182
45	1.2333	7.8347	3.3375	C	0.0349
46	6.1661	3.5633	3.3524	C	0.0341
47	6.1661	7.8349	3.3351	C	0.0331
48	1.2335	3.563	3.3511	C	0.0335
49	2.4665	0.0026	3.3405	C	-0.0479
50	2.4664	4.2751	3.3478	C	-0.0444
51	7.3993	0.0026	3.3404	C	-0.0478
52	7.3993	4.2751	3.3478	C	-0.0446
53	2.4664	1.4268	3.3498	C	0.0313
54	2.4667	5.6988	3.3383	C	0.0331
55	7.3994	1.4268	3.3498	C	0.0313
56	7.399	5.6988	3.3383	C	0.0331
57	3.6998	6.4109	3.3327	C	-0.0422
58	8.6325	2.1388	3.3514	C	-0.0436
59	8.6322	6.4106	3.3376	C	-0.0437
60	3.6992	2.1395	3.355	C	-0.0182
61	8.6325	7.8347	3.3375	C	0.0348
62	3.6997	3.5633	3.3523	C	0.034
63	3.6997	7.8349	3.3352	C	0.0331
64	8.6323	3.563	3.3511	C	0.0335
65	0.0007	4.2503	6.6444	C	0.0025
66	4.9337	8.5189	6.6405	C	-0.0454
67	0.0008	8.5225	6.61	C	0.0199
68	6.1677	0.6774	6.6725	C	0.0549
69	1.2398	0.6955	6.6406	C	0.0107
70	1.2851	4.954	6.6102	C	-0.0153
71	1.2589	2.1293	6.6934	C	0.0048
72	1.2473	6.3787	6.5625	C	-0.0053
73	6.154	2.0611	6.8824	C	0.3393
74	6.141	6.3953	6.5388	C	0.0186
75	4.9337	7.1412	6.553	C	0.0278
76	0.0008	2.8341	6.6705	C	-0.0008
77	0.0009	7.092	6.5698	C	0.0104
78	7.2807	4.2607	6.6489	C	0.0323
79	7.4038	8.5191	6.5893	C	0.0114
80	2.5867	4.2606	6.649	C	0.0331
81	2.4636	8.5192	6.5895	C	0.0114
82	8.6275	0.6955	6.6404	C	0.0103
83	8.5821	4.954	6.6102	C	-0.0157
84	3.6997	0.6774	6.6725	C	0.0553
85	8.6202	6.3787	6.5623	C	-0.0049
86	3.7266	6.3953	6.5389	C	0.0195
87	3.7134	2.0612	6.8824	C	0.3372
88	8.6083	2.1293	6.6934	C	0.0043
89	2.4718	7.0947	6.5475	C	0.0077
90	7.3957	7.0947	6.5473	C	0.008
91	2.5155	2.8314	6.7711	C	0.0341
92	7.3519	2.8314	6.7711	C	0.0342
93	6.0288	5.0136	6.5567	C	-0.0242
94	3.8388	5.0135	6.5568	C	-0.0519
95	4.9338	2.6158	7.3032	N	-0.5241
96	4.9339	3.6225	8.1211	O	-0.4684

2-HYDROXYPYRIDINE-NP

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	4.9329	8.5427	0.0107	C	-0.0215
2	0.0001	4.2707	0.0107	C	-0.0213
3	0.0001	8.5427	0.0107	C	-0.0213
4	4.9329	4.2707	0.0106	C	-0.0218
5	6.1662	0.7107	0.0099	C	0.036
6	1.2333	4.9827	0.0099	C	0.0362
7	6.1662	4.9827	0.0098	C	0.0361
8	1.2333	0.7107	0.0098	C	0.0362
9	1.2334	6.4067	0.0103	C	-0.0471
10	6.1663	2.1347	0.0103	C	-0.0472
11	1.2334	2.1347	0.0102	C	-0.047

12	6.1663	6.4067	0.0101	C	-0.0472
13	0.0001	2.8467	0.0102	C	0.0624
14	0.0001	7.1187	0.0102	C	0.0624
15	4.933	2.8467	0.0101	C	0.062
16	4.9329	7.1187	0.0101	C	0.0622
17	7.3994	4.2708	0.0106	C	-0.0511
18	2.4665	8.5428	0.0107	C	-0.0509
19	2.4665	4.2707	0.0106	C	-0.0511
20	7.3994	8.5427	0.0107	C	-0.0508
21	8.6326	0.7107	0.0099	C	0.036
22	3.6997	0.7107	0.0099	C	0.0359
23	8.6326	4.9827	0.0099	C	0.036
24	3.6997	4.9827	0.0097	C	0.036
25	3.6996	2.1347	0.0102	C	-0.0475
26	3.6996	6.4067	0.0102	C	-0.0475
27	8.6325	2.1347	0.0103	C	-0.047
28	8.6325	6.4067	0.0103	C	-0.047
29	7.3994	2.8469	0.0099	C	0.0319
30	2.4665	2.8469	0.0098	C	0.0323
31	7.3994	7.1188	0.0099	C	0.032
32	2.4665	7.1189	0.0099	C	0.0324
33	4.9327	0.0007	3.3502	C	-0.0237
34	9.8654	0.0014	3.3523	C	-0.0184
35	4.9329	4.2731	3.3494	C	-0.0338
36	9.8657	4.2733	3.3517	C	-0.0193
37	4.9325	1.4251	3.3495	C	0.0586
38	9.8656	5.6974	3.3515	C	0.0615
39	4.9331	5.6972	3.3483	C	0.0533
40	9.8656	1.4257	3.3514	C	0.0616
41	6.1665	6.409	3.3486	C	-0.0472
42	1.2332	2.1376	3.3503	C	-0.042
43	1.233	6.4094	3.3505	C	-0.0459
44	6.1661	2.1372	3.3496	C	-0.0516
45	1.233	7.8332	3.3513	C	0.0352
46	6.1662	3.5613	3.3494	C	0.0283
47	6.1662	7.8328	3.3493	C	0.0357
48	1.233	3.5613	3.3493	C	0.0374
49	7.3993	0.0013	3.3509	C	-0.0505
50	2.4662	0.0012	3.3513	C	-0.0486
51	7.3996	4.2735	3.3506	C	-0.0496
52	2.466	4.2732	3.3491	C	-0.0503
53	7.3996	5.6971	3.3491	C	0.0335
54	2.4662	5.6969	3.3485	C	0.0326
55	7.3994	1.425	3.3505	C	0.0316
56	2.4661	1.4251	3.3501	C	0.0352
57	8.6323	6.4093	3.3513	C	-0.0449
58	3.699	2.1369	3.3493	C	-0.0478
59	8.6324	2.1375	3.3508	C	-0.0448
60	3.6995	6.4088	3.3481	C	-0.0486
61	8.6325	7.8333	3.3514	C	0.0356
62	8.6325	3.5615	3.351	C	0.0352
63	3.6994	3.561	3.3491	C	0.0293
64	3.6994	7.8328	3.3493	C	0.0356
65	0.0961	0.2075	6.6999	C	0.0407
66	5.0546	8.3262	6.7009	C	0.0012
67	9.7441	4.3926	6.6965	C	-0.0103
68	1.3779	0.9395	6.7025	C	0.0131
69	6.2067	0.682	6.7016	C	0.0463
70	1.1404	5.0056	6.6991	C	0.0154
71	6.1482	2.1633	6.702	C	0.0161
72	6.4055	6.147	6.7014	C	-0.1437
73	1.3011	2.4795	6.7013	C	0.018
74	1.2656	6.4324	6.6994	C	-0.0065
75	0.0895	7.2744	6.6984	C	-0.0375
76	4.8224	2.6502	6.7003	C	1.0922
77	5.0683	6.7873	6.7041	C	-0.0068
78	9.8144	2.9835	6.6996	C	0.0335
79	7.458	0.0375	6.7	C	0.0317
80	2.1633	3.9953	6.702	C	0.0252
81	7.25	4.6578	6.7009	C	-0.2149
82	2.5448	8.5229	6.7002	C	0.0278
83	3.8356	0.5399	6.6985	C	0.5548
84	8.5865	5.1504	6.6972	C	0.0147
85	3.4596	4.6556	6.7037	C	0.4346
86	8.6557	0.8499	6.7002	C	-0.01
87	8.7384	6.5665	6.6965	C	0.0169
88	3.7043	6.1619	6.7029	C	-0.0236
89	8.5623	2.3088	6.7005	C	-0.0118
90	7.2697	3.0902	6.703	C	0.0076
91	2.5335	7.0551	6.702	C	-0.0191
92	7.472	7.1512	6.699	C	-0.0331
93	5.5405	4.5697	6.6919	H	0.6486
94	3.7878	1.8893	6.6944	N	-1.286
95	4.6646	4.0095	6.7019	O	-1.2064

2-PYRIDONE-NT

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	4.9329	8.5427	0.0107	C	-0.0216
2	0.0001	4.2707	0.0107	C	-0.0214
3	0.0001	8.5427	0.0107	C	-0.0214
4	4.9329	4.2707	0.0106	C	-0.0217
5	6.1662	0.7107	0.0099	C	0.036
6	1.2333	4.9827	0.0099	C	0.0362
7	6.1662	4.9827	0.0098	C	0.0363
8	1.2333	0.7107	0.0098	C	0.0361
9	1.2334	6.4067	0.0103	C	-0.0472
10	6.1663	2.1347	0.0103	C	-0.0471
11	1.2334	2.1347	0.0102	C	-0.0471
12	6.1663	6.4067	0.0101	C	-0.047
13	0.0001	2.8467	0.0102	C	0.0624
14	0.0001	7.1187	0.0102	C	0.0624
15	4.933	2.8467	0.0101	C	0.062
16	4.9329	7.1187	0.0101	C	0.0622
17	7.3994	4.2708	0.0106	C	-0.0509
18	2.4665	8.5428	0.0107	C	-0.051
19	2.4665	4.2707	0.0106	C	-0.0511
20	7.3994	8.5427	0.0107	C	-0.0508
21	8.6326	0.7107	0.0099	C	0.036
22	3.6997	0.7107	0.0099	C	0.0359
23	8.6326	4.9827	0.0099	C	0.0362
24	3.6997	4.9827	0.0097	C	0.036
25	3.6996	2.1347	0.0102	C	-0.0476
26	3.6996	6.4067	0.0102	C	-0.0474
27	8.6325	2.1347	0.0103	C	-0.0471
28	8.6325	6.4067	0.0103	C	-0.047
29	7.3994	2.8469	0.0099	C	0.0321
30	2.4665	2.8469	0.0098	C	0.0321
31	7.3994	7.1188	0.0099	C	0.0321
32	2.4665	7.1189	0.0099	C	0.0323
33	4.9327	0.0007	3.3502	C	-0.0255
34	9.8654	0.0014	3.3523	C	-0.0195
35	4.9329	4.2731	3.3494	C	-0.0213
36	9.8657	4.2733	3.3517	C	-0.0193
37	4.9325	1.4251	3.3495	C	0.0543
38	9.8656	5.6974	3.3515	C	0.0619
39	4.9331	5.6972	3.3483	C	0.0623
40	9.8656	1.4257	3.3514	C	0.061
41	6.1665	6.409	3.3486	C	-0.0445
42	1.2332	2.1376	3.3503	C	-0.0461
43	1.233	6.4094	3.3505	C	-0.0467
44	6.1661	2.1372	3.3496	C	-0.049
45	1.233	7.8332	3.3513	C	0.0345
46	6.1662	3.5613	3.3494	C	0.0347
47	6.1662	7.8328	3.3493	C	0.0368
48	1.233	3.5613	3.3493	C	0.0349
49	7.3993	0.0013	3.3509	C	-0.0503
50	2.4662	0.0012	3.3513	C	-0.0516
51	7.3996	4.2735	3.3506	C	-0.0468
52	2.466	4.2732	3.3491	C	-0.0518
53	7.3996	5.6971	3.3491	C	0.0362
54	2.4662	5.6969	3.3485	C	0.032
55	7.3994	1.425	3.3505	C	0.0312
56	2.4661	1.4251	3.3501	C	0.0273
57	8.6323	6.4093	3.3513	C	-0.0443
58	3.699	2.1369	3.3493	C	-0.0562
59	8.6324	2.1375	3.3508	C	-0.0444
60	3.6995	6.4088	3.3481	C	-0.049
61	8.6325	7.8333	3.3514	C	0.036
62	8.6325	3.5615	3.351	C	0.0362
63	3.6994	3.561	3.3491	C	0.0266
64	3.6994	7.8328	3.3493	C	0.0355
65	0.0961	0.2075	6.6999	C	0.0246
66	5.0546	8.3262	6.7009	C	0.0467
67	9.7441	4.3926	6.6965	C	-0.0186
68	1.3779	0.9395	6.7025	C	-0.0304
69	6.2067	0.682	6.7016	C	0.0408
70	1.1404	5.0056	6.6991	C	0.0202
71	6.1482	2.1633	6.702	C	0.0033
72	6.4055	6.147	6.7014	C	0.0017
73	1.3011	2.4795	6.7013	C	-0.1274
74	1.2656	6.4324	6.6994	C	-0.0065
75	0.0895	7.2744	6.6984	C	-0.0421
76	4.8224	2.6502	6.7003	C	1.1656
77	5.0683	6.7873	6.7041	C	-0.0141

78	9.8144	2.9835	6.6996	C	0.048
79	7.458	0.0375	6.7	C	-0.0412
80	2.1633	3.9953	6.702	C	-0.0737
81	7.25	4.6578	6.7009	C	-0.017
82	2.5448	8.5229	6.7002	C	0.0048
83	3.8356	0.5399	6.6985	C	0.4319
84	8.5865	5.1504	6.6972	C	0.0051
85	3.4596	4.6556	6.7037	C	0.5305
86	8.6557	0.8499	6.7002	C	0.0131
87	8.7384	6.5665	6.6965	C	0.0109
88	3.7043	6.1619	6.7029	C	-0.0049
89	8.5623	2.3088	6.7005	C	-0.012
90	7.2697	3.0902	6.703	C	0.0155
91	2.5335	7.0551	6.702	C	0.0416
92	7.472	7.1512	6.699	C	0.0054
93	2.8804	2.3432	6.6909	H	0.4951
94	3.7878	1.8893	6.6944	N	-1.3864
95	4.6646	4.0095	6.7019	O	-1.1049

QUATERNARY NITROGEN-Q2

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	9.8657	8.543	0.014	C	-0.0229
2	0	4.271	0.014	C	-0.0229
3	4.9329	8.5429	0.0143	C	-0.0231
4	4.9329	4.2709	0.0143	C	-0.0231
5	1.2333	0.7108	0.013	C	0.0341
6	1.2332	4.9828	0.0129	C	0.0343
7	6.1662	0.7108	0.0131	C	0.0342
8	6.1662	4.9829	0.0132	C	0.0342
9	1.2334	2.135	0.0128	C	-0.049
10	1.2333	6.407	0.0127	C	-0.0491
11	6.1662	2.1349	0.013	C	-0.049
12	6.1663	6.4069	0.013	C	-0.0491
13	9.8657	2.8468	0.013	C	0.061
14	0	7.1188	0.013	C	0.061
15	4.9329	2.8468	0.0134	C	0.0606
16	4.9329	7.1188	0.0134	C	0.0606
17	7.3993	8.5429	0.0137	C	-0.0522
18	7.3993	4.2709	0.0139	C	-0.052
19	2.4664	8.5429	0.0139	C	-0.052
20	2.4664	4.2709	0.0137	C	-0.0522
21	8.6325	0.7108	0.0129	C	0.0343
22	8.6325	4.9828	0.013	C	0.0341
23	3.6996	0.7109	0.0132	C	0.0342
24	3.6996	4.9828	0.0131	C	0.0342
25	3.6995	2.1349	0.013	C	-0.0491
26	3.6995	6.4069	0.013	C	-0.049
27	8.6324	2.135	0.0127	C	-0.0491
28	8.6324	6.407	0.0128	C	-0.049
29	7.3994	7.1191	0.0126	C	0.0313
30	7.3993	2.847	0.0126	C	0.0311
31	2.4664	7.119	0.0126	C	0.0311
32	2.4664	2.8471	0.0126	C	0.0313
33	4.933	0.0009	3.353	C	-0.0274
34	4.9328	4.2729	3.353	C	-0.0274
35	9.8657	0.0008	3.352	C	-0.0235
36	0.0001	4.2728	3.352	C	-0.0235
37	9.8657	1.4248	3.3521	C	0.061
38	0	5.6968	3.3521	C	0.061
39	4.933	1.4251	3.3531	C	0.0546
40	4.9327	5.6971	3.3531	C	0.0546
41	6.1666	2.1367	3.352	C	-0.0506
42	6.1662	6.409	3.3527	C	-0.0526
43	1.2332	2.1369	3.3519	C	-0.0496
44	1.2332	6.4086	3.3514	C	-0.0496
45	6.1664	3.5607	3.3533	C	0.0314
46	6.1664	7.8331	3.3527	C	0.0326
47	1.2331	3.5608	3.3519	C	0.034
48	1.2328	7.8326	3.3522	C	0.0352
49	2.4661	0.0007	3.3531	C	-0.0568
50	2.4663	4.2728	3.3519	C	-0.0534
51	7.3994	0.0008	3.3519	C	-0.0534
52	7.3996	4.2727	3.3531	C	-0.0568
53	7.3996	5.6969	3.3531	C	0.0274
54	2.4661	1.4249	3.3531	C	0.0274
55	2.4662	5.6966	3.3517	C	0.0307
56	7.3996	1.4246	3.3517	C	0.0307
57	8.6325	2.1366	3.3514	C	-0.0496
58	3.6992	6.4087	3.352	C	-0.0506
59	3.6995	2.137	3.3527	C	-0.0527

60	8.6326	6.4089	3.3519	C	-0.0496
61	3.6994	3.5611	3.3527	C	0.0326
62	3.6994	7.8327	3.3533	C	0.0314
63	8.6326	7.8328	3.3519	C	0.034
64	8.6329	3.5606	3.3522	C	0.0352
65	0.003	0.0009	6.6973	C	-0.0159
66	4.9367	4.271	6.6922	C	0.3255
67	4.929	8.543	6.6922	C	0.3255
68	9.8627	4.2729	6.6973	C	-0.0159
69	6.1552	0.7176	6.6962	C	-0.0105
70	1.2444	0.7142	6.6962	C	-0.0212
71	1.2372	4.9843	6.6996	C	-0.035
72	6.1631	6.4031	6.6918	C	0.3401
73	1.2303	2.1373	6.6958	C	0.038
74	6.1695	2.1338	6.695	C	0.0533
75	1.2366	6.4117	6.6987	C	0.0183
76	4.9298	7.1212	6.6935	C	0.0541
77	4.936	2.8492	6.6935	C	0.0541
78	9.8645	7.1188	6.6984	C	0.0692
79	0.0013	2.8468	6.6984	C	0.0692
80	2.4762	4.2651	6.6981	C	-0.0264
81	7.3897	4.2798	6.6939	C	0.3298
82	7.3896	8.5371	6.6981	C	-0.0264
83	2.4761	0.0078	6.6939	C	0.3297
84	3.7105	4.9896	6.6962	C	-0.0105
85	8.6214	4.9862	6.6962	C	-0.0212
86	8.6286	0.7123	6.6996	C	-0.035
87	3.7027	2.1311	6.6918	C	0.34
88	3.6962	6.4058	6.695	C	0.0533
89	8.6355	6.4093	6.6958	C	0.038
90	8.6292	2.1397	6.6987	C	0.0183
91	2.4721	2.8384	6.6956	C	0.0591
92	2.4764	7.1278	6.6973	C	0.0574
93	7.3936	7.1104	6.6956	C	0.0591
94	7.3893	2.8558	6.6973	C	0.0574
95	6.1628	4.986	6.6923	N	-1.1536
96	3.7029	0.714	6.6923	N	-1.1536

QUATERNARY NITROGEN-Q4

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	9.8658	4.272	0.0003	C	-0.0271
2	4.9329	0	0.0003	C	-0.0271
3	0	0	0.0003	C	-0.0271
4	4.9329	4.272	0.0003	C	-0.0271
5	6.1661	0.7119	0.0002	C	0.0369
6	1.2332	0.7119	0.0002	C	0.0369
7	1.2332	4.9839	0.0002	C	0.0369
8	6.1661	4.9839	0.0002	C	0.0369
9	1.2332	2.136	0.0003	C	-0.052
10	1.2332	6.408	0.0003	C	-0.052
11	6.1661	2.136	0.0003	C	-0.052
12	6.1661	6.408	0.0003	C	-0.052
13	9.8658	2.8479	0.0002	C	0.0625
14	0	7.1199	0.0002	C	0.0625
15	4.9329	2.8479	0.0002	C	0.0625
16	4.9329	7.1199	0.0002	C	0.0625
17	7.3993	4.272	0.0003	C	-0.0544
18	2.4664	0	0.0003	C	-0.0544
19	2.4664	4.272	0.0003	C	-0.0544
20	7.3993	0	0.0003	C	-0.0544
21	3.6997	4.9839	0.0002	C	0.0369
22	8.6325	0.7119	0.0002	C	0.0369
23	8.6325	4.9839	0.0002	C	0.0369
24	3.6997	0.7119	0.0002	C	0.0369
25	3.6997	2.136	0.0003	C	-0.052
26	3.6997	6.408	0.0003	C	-0.052
27	8.6325	2.136	0.0003	C	-0.052
28	8.6325	6.408	0.0003	C	-0.052
29	2.4664	7.1199	0.0002	C	0.034
30	7.3993	7.1199	0.0002	C	0.034
31	2.4664	2.8479	0.0002	C	0.034
32	7.3993	2.8479	0.0002	C	0.034
33	9.8657	4.2719	3.3501	C	-0.0278
34	4.933	8.5439	3.3501	C	-0.0278
35	4.9328	4.2719	3.3501	C	-0.0278
36	0.0001	8.5439	3.3501	C	-0.0278
37	4.933	1.4242	3.3502	C	0.0596
38	0.0001	1.4242	3.3502	C	0.0596
39	9.8657	5.6962	3.3502	C	0.0596
40	4.9328	5.6962	3.3502	C	0.0596
41	6.1661	6.408	3.3499	C	-0.0536
42	1.2332	2.1359	3.3498	C	-0.0518

43	1.2332	6.408	3.3499	C	-0.0536
44	6.1661	2.1359	3.3498	C	-0.0518
45	1.2332	7.8321	3.3501	C	0.0363
46	6.1661	3.5599	3.3501	C	0.0349
47	6.1661	7.8321	3.3501	C	0.0363
48	1.2332	3.5599	3.3501	C	0.0349
49	2.4664	8.5439	3.3501	C	-0.0595
50	2.4665	4.2719	3.3501	C	-0.0594
51	7.3992	8.5439	3.3501	C	-0.0595
52	7.3994	4.2719	3.3501	C	-0.0594
53	7.3994	5.6962	3.3502	C	0.0288
54	2.4665	5.6962	3.3502	C	0.0288
55	7.3992	1.4242	3.3502	C	0.0289
56	2.4663	1.4242	3.3502	C	0.0289
57	8.6325	6.4079	3.3498	C	-0.0518
58	8.6325	2.136	3.3499	C	-0.0536
59	3.6997	6.4079	3.3498	C	-0.0518
60	3.6997	2.136	3.3499	C	-0.0536
61	3.6997	7.8319	3.3501	C	0.0349
62	3.6997	3.5601	3.3501	C	0.0363
63	8.6325	7.8319	3.3501	C	0.0349
64	8.6325	3.5601	3.3501	C	0.0363
65	0.0004	8.5437	6.7102	C	0.3282
66	4.9324	4.2717	6.7102	C	0.3282
67	4.9333	8.5437	6.7102	C	0.3282
68	9.8653	4.2717	6.7102	C	0.3282
69	6.1661	0.7169	6.7119	C	0.0169
70	1.2332	0.7169	6.7119	C	0.0169
71	1.2332	6.4091	6.7102	C	0.3347
72	6.1661	6.4091	6.7102	C	0.3347
73	1.2332	2.1362	6.7103	C	0.0721
74	6.1661	2.1362	6.7103	C	0.0721
75	0.0041	2.846	6.7119	C	0.0518
76	4.9287	7.118	6.7119	C	0.0518
77	4.937	2.846	6.7119	C	0.0518
78	9.8616	7.118	6.7119	C	0.0518
79	7.3989	8.5437	6.7102	C	0.3403
80	2.4669	4.2717	6.7102	C	0.3403
81	7.3998	4.2717	6.7102	C	0.3403
82	2.466	8.5437	6.7102	C	0.3403
83	3.6997	4.9889	6.7119	C	0.0168
84	8.6325	4.9889	6.7119	C	0.0168
85	3.6997	6.4082	6.7103	C	0.0721
86	8.6325	2.1371	6.7102	C	0.3347
87	3.6997	2.1371	6.7102	C	0.3347
88	8.6325	6.4082	6.7103	C	0.0721
89	7.3952	2.846	6.7119	C	0.0281
90	2.4706	7.118	6.7119	C	0.0281
91	7.4035	7.118	6.7119	C	0.0281
92	2.4623	2.846	6.7119	C	0.0281
93	1.2332	4.9838	6.7117	N	-1.1237
94	6.1661	4.9838	6.7117	N	-1.1237
95	3.6997	0.7118	6.7117	N	-1.1237
96	8.6325	0.7118	6.7117	N	-1.1237

QUATERNARY NITROGEN-Q6

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	4.9328	8.5434	0.0078	C	-0.0246
2	9.8657	8.5434	0.0078	C	-0.0246
3	9.8657	4.2714	0.0078	C	-0.0246
4	4.9328	4.2714	0.0078	C	-0.0246
5	1.2332	4.9832	0.0076	C	0.0354
6	6.1661	0.7112	0.0076	C	0.0352
7	1.2332	0.7112	0.0076	C	0.0352
8	6.1661	4.9832	0.0076	C	0.0354
9	1.2333	2.1354	0.0083	C	-0.0498
10	1.2333	6.4075	0.0082	C	-0.0497
11	6.1661	2.1354	0.0083	C	-0.0498
12	6.1662	6.4075	0.0082	C	-0.0497
13	9.8656	2.8472	0.0078	C	0.0605
14	9.8657	7.1192	0.0077	C	0.0603
15	4.9328	2.8472	0.0078	C	0.0605
16	4.9328	7.1192	0.0077	C	0.0603
17	2.4663	8.5434	0.0085	C	-0.0531
18	2.4663	4.2714	0.0086	C	-0.0533
19	7.3992	8.5434	0.0085	C	-0.0531
20	7.3992	4.2714	0.0086	C	-0.0533
21	3.6995	0.7112	0.0075	C	0.0355
22	3.6996	4.9832	0.0075	C	0.0355
23	8.6324	0.7112	0.0075	C	0.0355

24	8.6324	4.9832	0.0075	C	0.0355
25	3.6994	2.1354	0.0083	C	-0.0493
26	3.6994	6.4075	0.0082	C	-0.0491
27	8.6323	2.1354	0.0083	C	-0.0493
28	8.6323	6.4075	0.0082	C	-0.0491
29	2.4663	2.8474	0.0082	C	0.0315
30	2.4663	7.1193	0.008	C	0.0315
31	7.3992	2.8474	0.0082	C	0.0315
32	7.3992	7.1193	0.008	C	0.0315
33	9.8654	0.0003	3.351	C	-0.0266
34	9.8653	4.2726	3.3512	C	-0.025
35	4.9326	0.0003	3.351	C	-0.0266
36	4.9325	4.2726	3.3512	C	-0.025
37	9.8653	5.6969	3.3498	C	0.0583
38	4.9328	1.4243	3.3514	C	0.0599
39	9.8657	1.4243	3.3514	C	0.0599
40	4.9324	5.6969	3.3498	C	0.0583
41	1.233	2.1363	3.3503	C	-0.0531
42	1.2331	6.4085	3.3495	C	-0.0517
43	6.1659	2.1363	3.3503	C	-0.0531
44	6.166	6.4085	3.3495	C	-0.0517
45	1.2328	3.5605	3.3522	C	0.0304
46	1.2329	7.8325	3.3503	C	0.0364
47	6.1657	3.5605	3.3522	C	0.0304
48	6.1658	7.8325	3.3503	C	0.0364
49	2.466	8.544	3.3511	C	-0.0578
50	2.4662	4.2724	3.3523	C	-0.0568
51	7.3989	8.544	3.3511	C	-0.0578
52	7.399	4.2724	3.3523	C	-0.0568
53	7.3988	1.4242	3.3517	C	0.0278
54	2.466	1.4242	3.3517	C	0.0278
55	7.3991	5.6969	3.3502	C	0.0284
56	2.4663	5.6969	3.3502	C	0.0284
57	3.6992	2.1364	3.3515	C	-0.0546
58	8.6319	6.4083	3.3484	C	-0.0494
59	8.6321	2.1364	3.3515	C	-0.0546
60	3.699	6.4083	3.3484	C	-0.0494
61	8.6323	3.5606	3.352	C	0.0323
62	3.6992	7.8323	3.3503	C	0.0341
63	3.6994	3.5606	3.352	C	0.0323
64	8.6321	7.8323	3.3503	C	0.0341
65	4.9346	4.2759	6.704	C	0.299
66	0.0009	0.0071	6.7019	C	0.3322
67	4.9338	0.0071	6.7019	C	0.3322
68	0.0017	4.2759	6.704	C	0.299
69	1.2385	0.7236	6.7046	C	0.07
70	6.1714	0.7236	6.7046	C	0.07
71	1.2358	6.4054	6.7024	C	0.3181
72	6.1687	6.4054	6.7024	C	0.3181
73	1.2352	2.1386	6.7044	C	0.2932
74	6.1681	2.1386	6.7044	C	0.2932
75	0.0048	2.8491	6.7052	C	0.099
76	4.9277	7.1179	6.7048	C	0.0629
77	4.9377	2.8491	6.7052	C	0.099
78	9.8606	7.1179	6.7048	C	0.0629
79	2.4705	4.2674	6.7012	C	0.752
80	7.4034	4.2674	6.7012	C	0.752
81	2.4604	8.5404	6.7034	C	0.3279
82	7.3933	8.5404	6.7034	C	0.3279
83	3.7003	4.9795	6.7056	C	0.044
84	8.6332	4.9795	6.7056	C	0.044
85	8.6274	6.4041	6.7054	C	0.0567
86	3.6945	6.4041	6.7054	C	0.0567
87	8.6344	2.1429	6.6982	C	0.7641
88	3.7016	2.1429	6.6982	C	0.7641
89	2.4694	7.1185	6.7047	C	0.0469
90	7.4023	7.1185	6.7047	C	0.0469
91	1.2402	4.9689	6.7001	N	-1.1308
92	6.1731	4.9689	6.7001	N	-1.1308
93	8.6235	0.725	6.697	N	-1.1142
94	3.6906	0.725	6.697	N	-1.1142
95	7.3981	2.8453	6.6971	N	-1.1255
96	2.4652	2.8453	6.6971	N	-1.1255

QUATERNARY NITROGEN-Q8

COORDINATES (ANGSTROM)

ATOM	X	Y	Z	SYMBOL	Q
1	0	0	0.0003	C	-0.027
2	9.8658	4.272	0.0003	C	-0.027
3	4.9329	0	0.0003	C	-0.027
4	4.9329	4.272	0.0003	C	-0.027
5	1.2332	0.7119	0.0002	C	0.037
6	1.2332	4.9839	0.0002	C	0.0369

7	6.1661	0.7119	0.0002	C	0.037
8	6.1661	4.9839	0.0002	C	0.0369
9	1.2332	2.136	0.0003	C	-0.0521
10	1.2332	6.408	0.0003	C	-0.0521
11	6.1661	2.136	0.0003	C	-0.0521
12	6.1661	6.408	0.0003	C	-0.0521
13	9.8658	2.8479	0.0002	C	0.0625
14	0	7.1199	0.0002	C	0.0625
15	4.9329	2.8479	0.0002	C	0.0625
16	4.9329	7.1199	0.0002	C	0.0625
17	2.4664	4.272	0.0003	C	-0.0545
18	7.3993	0	0.0003	C	-0.0545
19	7.3993	4.272	0.0003	C	-0.0545
20	2.4664	0	0.0003	C	-0.0545
21	8.6325	4.9839	0.0002	C	0.037
22	3.6997	0.7119	0.0002	C	0.0369
23	3.6997	4.9839	0.0002	C	0.037
24	8.6325	0.7119	0.0002	C	0.0369
25	3.6997	2.136	0.0003	C	-0.0521
26	3.6997	6.408	0.0003	C	-0.0521
27	8.6325	2.136	0.0003	C	-0.0521
28	8.6325	6.408	0.0003	C	-0.0521
29	7.3993	2.8479	0.0002	C	0.0339
30	2.4664	2.8479	0.0002	C	0.0339
31	7.3993	7.1199	0.0002	C	0.0339
32	2.4664	7.1199	0.0002	C	0.0339
33	4.9327	4.2718	3.3499	C	-0.0272
34	0.0001	8.544	3.35	C	-0.0288
35	9.8656	4.2718	3.3499	C	-0.0272
36	4.933	8.544	3.35	C	-0.0288
37	0.0001	1.4242	3.35	C	0.0611
38	9.8656	5.696	3.3501	C	0.0591
39	4.933	1.4242	3.35	C	0.0611
40	4.9327	5.696	3.3501	C	0.0591
41	1.2333	6.408	3.35	C	-0.0554
42	6.166	2.1358	3.3499	C	-0.0531
43	6.1662	6.408	3.35	C	-0.0554
44	1.2331	2.1358	3.3499	C	-0.0531
45	6.1662	7.8322	3.35	C	0.0351
46	1.2331	3.56	3.3501	C	0.0339
47	1.2334	7.8322	3.35	C	0.0351
48	6.1659	3.56	3.3501	C	0.0339
49	2.4663	8.5438	3.3499	C	-0.0586
50	2.4665	4.272	3.35	C	-0.0605
51	7.3992	8.5438	3.3499	C	-0.0586
52	7.3994	4.272	3.35	C	-0.0605
53	7.3995	5.6962	3.35	C	0.0302
54	2.4666	5.6962	3.35	C	0.0302
55	7.3992	1.424	3.3501	C	0.0287
56	2.4663	1.424	3.3501	C	0.0287
57	3.6995	6.4078	3.3499	C	-0.0526
58	3.6997	2.136	3.35	C	-0.0553
59	8.6324	6.4078	3.3499	C	-0.0526
60	8.6326	2.136	3.35	C	-0.0553
61	8.6324	7.832	3.3501	C	0.0336
62	8.6327	3.5602	3.35	C	0.0351
63	3.6995	7.832	3.3501	C	0.0336
64	3.6998	3.5602	3.35	C	0.0351
65	0.0039	0.0024	6.71	C	0.7302
66	4.9298	4.2702	6.7104	C	0.3017
67	4.9368	0.0024	6.71	C	0.7302
68	9.8627	4.2702	6.7104	C	0.3017
69	6.1694	0.7141	6.712	C	0.0993
70	1.2365	0.7141	6.712	C	0.0993
71	1.2372	6.4104	6.71	C	0.7228
72	6.17	6.4104	6.71	C	0.7228
73	1.2301	2.1342	6.7104	C	0.3053
74	6.163	2.1342	6.7104	C	0.3053
75	0.0033	2.8501	6.712	C	0.1077
76	4.9362	2.8501	6.712	C	0.1077
77	2.4704	4.2744	6.71	C	0.7225
78	7.4033	4.2744	6.71	C	0.7225
79	2.4634	8.5422	6.7104	C	0.3059
80	7.3962	8.5422	6.7104	C	0.3059
81	3.703	4.9861	6.712	C	0.1159
82	8.6358	4.9861	6.712	C	0.1159
83	3.6966	6.4062	6.7104	C	0.3011
84	3.7036	2.1384	6.71	C	0.7252
85	8.6295	6.4062	6.7104	C	0.3011
86	8.6365	2.1384	6.71	C	0.7252
87	7.4026	7.1221	6.712	C	0.103
88	2.4697	7.1221	6.712	C	0.103
89	1.2291	4.9819	6.7117	N	-1.1131
90	6.162	4.9819	6.7117	N	-1.1131

91	4.9288	7.1179	6.7117	N	-1.1005
92	9.8617	7.1179	6.7117	N	-1.1005
93	8.6285	0.7099	6.7117	N	-1.109
94	3.6956	0.7099	6.7117	N	-1.109
95	7.3952	2.8459	6.7117	N	-1.1121
96	2.4624	2.8459	6.7117	N	-1.1121

Building the slit-pore model

From the VASP-optimized models presented above, slit-pore models of varying width can be constructed from the following steps.

1. Transpose all coordinates along *x* so that the functionality centered on the surface becomes offset. This resolves unnatural functionality overlap in very narrow slit-pore models. (transpose can be an arbitrary amount, δ).

$(x_T,y,z) = ((x + \delta),y,z)$

2. Mirror the cell about a center of inversion, *i*, such that the functionality resides on opposites sides of the surface center. *x* and *y* coordinates can be transposed by the following relations:

$x_T = |x - 9.86576|$

$y_T = |y - 8.544|$

where 9.86576 and 8.544 are the unit cell dimensions along the *x* and *y* coordinate, respectively. Transpose of the *z* coordinates results in the mirror inversion of the transposed *xy* coordinates about a σ_h plane placed at the pore center. For a slit-pore with the desired pore width λ, it is first necessary to determine the maximum height of the total slit-pore model, measured as the difference in the least positive *z* coordinate to the most positive *z* coordinate. This is achieved by the following:

$cell\ height = max(z_i + \lambda + 16.65)$

where *i* runs over all *z* coordinates and the factor 16.65 represents the sum of the heights of both 3-layered graphitic models plus the kinetic collision diameter of carbon. Finally, the *z* coordinates can be transposed by the following:

$$z_T = cell\ height - z$$

3.The cell height is also used to set the edge cell length and the effective bound box size for GCMC simulations. An effective slit pore was simulated by setting periodicity in the *x* and *y* directions, while the *z* direction is held constant.

The previous steps are depicted schematically in Figure S4.

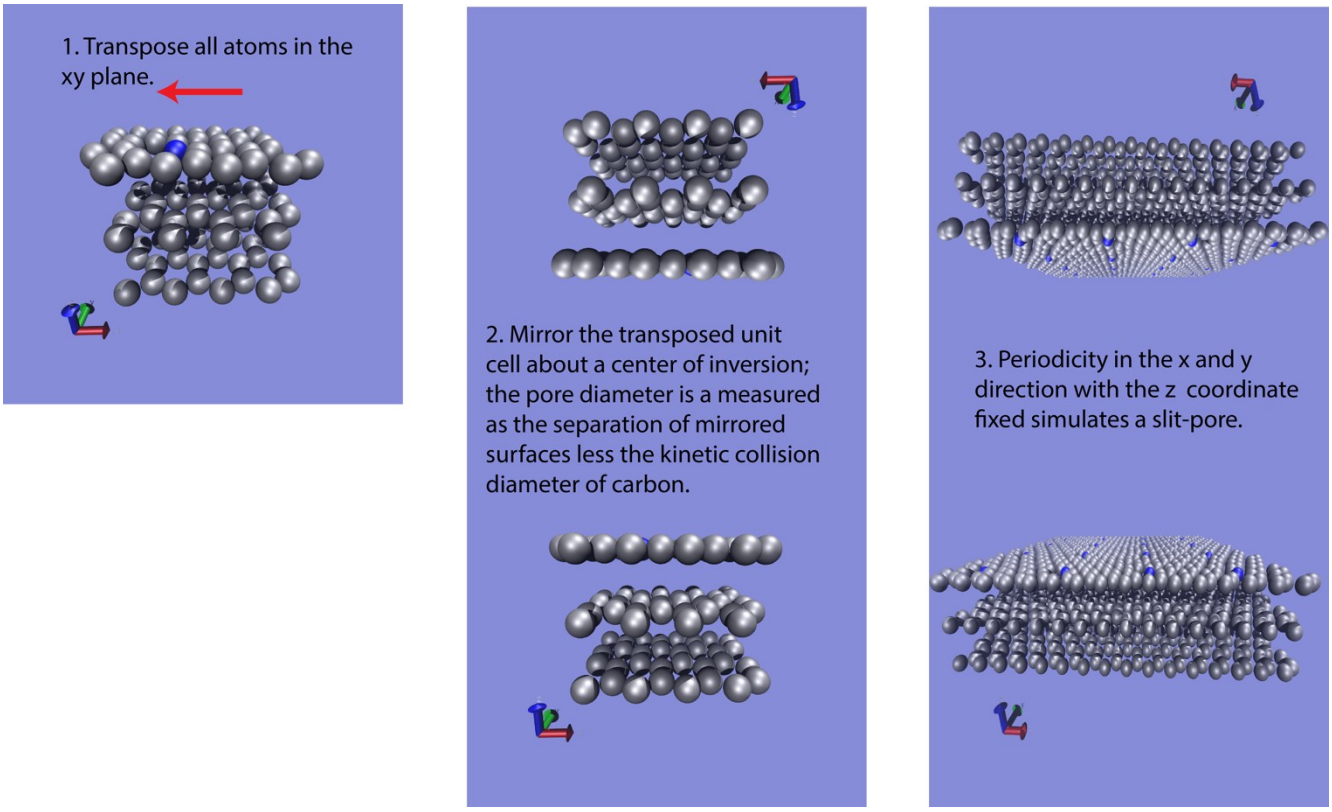

Figure S4. Schematic workflow for the creation of a slit-pore unit cell from a VASP optimized structure.

References

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