Electronic Supporting Information

CO_2 Adsorption in Natural Deep Eutectic Solvents: Insights from Quantum Mechanics and Molecular Dynamics

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Table S1. Calculated density and experimental density of different systems

(1A3G means the molar ratio of arginine to glycerol is 1 : 3)

	1A3G	1A4G	1A5G	1A6G	1A7G	1A8G	1A9G
Computation density g/cm^3	1.313	1.309	1.304	1.307	1.307	1.306	1.302
Experimental density g/cm^3	1.213	1.220	1.225	1.229	1.231	1.233	1.235
Deviation %	7.62	6.80	6.06	5.97	5.81	5.59	5.15

Table S2. General Amber force field parameters

Atom type	**Mass**	**Ptype**	**Sigma (nm)**	**Epsilon (kJ/mol)**
n3	14.01000	A	0.325000	0.711280
hn	1.00800	A	0.106908	0.0656888
c3	12.01000	A	0.339967	0.457730
h1	1.00800	A	0.247135	0.0656888
c	12.01000	A	0.339967	0.359824
hc	1.00800	A	0.264953	0.0656888
o	16.00000	A	0.295992	0.878640
nh	14.01000	A	0.325000	0.711280
c2	12.01000	A	0.339967	0.359824
n2	14.01000	A	0.325000	0.711280
oh	16.00000	A	0.306647	0.880314
ho	1.00800	A	0.000000	0.000000
c1	12.01000	A	0.339967	0.878640

Table S3. Parameters for arginine

Atom number	Atom type	Atom name	Coordination			Charge
			X	Y	Z	
1	n3	N1	3.630	-1.410	-0.380	-1.1133494944
2	hn	H1	3.660	-1.710	0.580	0.3932784391
3	c3	C1	2.520	-0.480	-0.590	0.4551817702
4	h1	H2	2.480	-0.240	-1.650	0.0286247581
5	c3	C2	1.150	-1.000	-0.130	-0.3333598985
6	c	C3	2.850	0.830	0.110	0.6690911117
7	hc	H3	0.980	-1.940	-0.680	0.0671924813
8	hc	H4	1.210	-1.260	0.930	0.0671924813
9	c3	C4	-0.000	-0.040	-0.390	0.0316707860
10	o	O1	2.840	1.920	-0.410	-0.6400469357
11	hc	H5	0.140	0.890	0.180	-0.0062928291
12	hc	H6	-0.020	0.240	-1.440	-0.0062928291
13	c3	C5	-1.340	-0.640	0.010	0.5218318787
14	h1	H7	-1.510	-1.580	-0.540	-0.0456828649
15	h1	H8	-1.350	-0.890	1.070	-0.0456828649
16	nh	N2	-2.420	0.300	-0.240	-0.8749807825
17	hn	H9	-2.330	0.840	-1.090	0.3995906341
18	c2	C6	-3.710	0.030	0.140	0.9443111678
19	n2	N3	-3.980	-0.990	0.890	-1.0460754223
20	nh	N4	-4.640	0.920	-0.390	-0.9445568904
21	hn	H10	-4.960	-0.990	1.140	0.3876142426
22	hn	H11	-4.310	1.850	-0.550	0.3822916574
23	hn	H12	-5.540	0.900	0.070	0.3868449243
24	hn	H13	3.480	-2.240	-0.950	0.4302925983
25	oh	O2	3.130	0.650	1.410	-0.5581123186
26	ho	H14	3.330	1.520	1.810	0.4494241993

Table S4. Parameters for glycerol

Atom number	Atom type	Atom name	Coordination			Charge
			X	Y	Z	
1	c3	C1	1.300	-0.520	0.340	0.1455517688
2	h1	H1	1.310	-1.600	0.150	0.0222339830
3	h1	H2	1.320	-0.350	1.420	0.0222339830
4	c3	C2	0.030	0.070	-0.230	0.3518624679
5	h1	H3	0.100	0.050	-1.330	0.0327516223
6	c3	C3	-1.190	-0.740	0.190	0.0686377814
7	h1	H4	-1.250	-0.790	1.280	0.0385488174
8	h1	H5	-1.130	-1.750	-0.210	0.0385488174
9	oh	O1	-0.100	1.420	0.210	-0.6625236346
10	ho	H6	-1.020	1.670	0.030	0.4027883631
11	oh	O2	-2.340	-0.060	-0.340	-0.6801729420
12	ho	H7	-3.120	-0.340	0.150	0.4609645072
13	oh	O3	2.420	0.110	-0.290	-0.6930086286
14	ho	H8	3.220	-0.250	0.110	0.4515830937

Table S5. Parameters for CO_2

Atom number	Atom type	Atom name	Coordination			Charge
			X	Y	Z	
1	o	O1	-1.950	0.530	-0.000	-0.3933990076
2	c1	C1	-0.800	0.530	0.000	0.7866953474
3	o	O2	0.360	0.530	-0.000	-0.3932963398

Table S6. Details of hydrogen bonds with occupancy > 80%.

(Residue ID 1 is arginine, Residue ID 2-201 are glycerol.)

Number	Atom ID		Atom Name		Residue ID	
	D	A	D	A	D	A
0.987	1506	0	O2	N1	107	1
0.968	2586	18	O3	N3	184	1
0.960	1394	18	O2	N3	99	1
0.817	0	2540	N1	O1	1	181
0.791	0	2794	N1	O2	1	199
0.768	15	2582	N2	O1	1	184

Table S7. Hydrogen bonds in 1A200G box.

Type	Doner	Acceptor	Occupancy
1	Gly-Side-O2	Arg-Side-N1	99.98%
2	Gly-Side-O3	Arg-Side-N3	99.90%
3	Gly-Side-O2	Arg-Side-N3	99.88%
4	Arg-Side-N1	Gly-Side-O1	96.10%
5	Arg-Side-N2	Gly-Side-O1	88.43%
6	Arg-Side-N4	Gly-Side-O2	88.00%
7	Arg-Side-N1	Gly-Side-O2	86.23%
8	Arg-Side-N3	Gly-Side-O2	78.26%
9	Gly-Side-O1	Arg-Side-O1	68.96%
10	Gly-Side-O2	Arg-Side-C6	64.38%
11	Arg-Side-O2	Gly-Side-O2	64.28%
12	Arg-Side-N4	Gly-Side-O3	51.79%
13	Gly-Side-O3	Arg-Side-C6	47.29%
14	Gly-Side-O1	Arg-Side-N4	30.44%
15	Arg-Side-N3	Gly-Side-C3	23.62%
16	Gly-Side-C3	Arg-Side-O1	20.47%
17	Ar-Side-O2	Gly-Side-O3	18.00%
18	Gly-Side-O1	Arg-Side-O2	16.20%
19	Gly-Side-O1	Arg-Side-C3	14.72%
20	Arg-Side-O2	Gly-Side-C1	11.75%
21	Arg-Side-N4	Gly-Side-C3	11.47%
22	Gly-Side-C3	Arg-Side-O2	9.80%
23	Arg-Side-N4	Gly-Side-O1	9.60%
24	Gly-Side-O3	Arg-Side-O1	8.50%
25	Gly-Side-C2	Arg-Side-O1	6.32%
26	Gly-Side-C1	Arg-Side-O1	6.02%
27	Gly-Side-O2	Arg-Side-N2	5.60%
28	Gly-Side-O2	Arg-Side-C1	5.10%
29	Gly-Side-O1	Arg-Side-N3	4.87%
30	Arg-Side-N4	Gly-Side-C1	4.50%
31	Arg-Side-C4	Gly-Side-O2	4.20%
32	Arg-Side-N1	Gly-Side-C3	3.87%
33	Arg-Side-O2	Gly-Side-C3	3.02%
34	Arg-Side-C5	Gly-Side-O1	2.95%
35	Arg-Side-C1	Gly-Side-O2	2.92%
36	Gly-Side-O1	Arg-Side-C6	2.82%
37	Arg-Side-C4	Gly-Side-O3	2.42%
38	Gly-Side-O3	Arg-Side-C3	2.12%
39	Arg-Side-C4	Gly-Side-O1	1.92%
40	Arg-Side-N1	Gly-Side-O3	1.60%

41	Gly-Side-O2	Arg-Side-N4	1.55%
42	Arg-Side-C5	Gly-Side-O3	1.55%
43	Arg-Side-C2	Gly-Side-O1	1.52%
44	Arg-Side-C5	Gly-Side-O2	1.32%
45	Gly-Side-C1	Arg-Side-N1	1.15%
46	Arg-Side-C2	Gly-Side-O2	0.92%
47	Arg-Side-C2	Gly-Side-O3	0.70%
48	Gly-Side-O3	Arg-Side-N2	0.60%
49	Gly-Side-C3	Arg-Side-N4	0.32%
50	Gly-Side-C1	Arg-Side-O2	0.30%
51	Gly-Side-O3	Arg-Side-N4	0.27%
52	Arg-Side-N2	Gly-Side-O2	0.27%
53	Gly-Side-C1	Arg-Side-N4	0.20%
54	Gly-Side-O3	Arg-Side-O2	0.15%
55	Gly-Side-C3	Arg-Side-C5	0.15%
56	Arg-Side-C1	Gly-Side-C3	0.15%
57	Arg-Side-C5	Gly-Side-C3	0.15%
58	Gly-Side-C3	Arg-Side-N3	0.15%
59	Arg-Side-C1	Gly-Side-O3	0.15%
60	Gly-Side-O1	Arg-Side-C4	0.15%
61	Gly-Side-O2	Arg-Side-O1	0.15%
62	Gly-Side-O1	Arg-Side-N2	0.10%
63	Gly-Side-C3	Arg-Side-N1	0.07%
64	Arg-Side-N4	Gly-Side-C2	0.07%
65	Arg-Side-C2	Gly-Side-C3	0.05%
66	Arg-Side-C5	Gly-Side-C1	0.05%
67	Arg-Side-N2	Gly-Side-C2	0.05%
68	Gly-Side-C1	Arg-Side-C6	0.05%
69	Gly-Side-O1	Arg-Side-C5	0.05%
70	Gly-Side-C2	Arg-Side-O2	0.02%
71	Gly-Side-O1	Arg-Side-N1	0.02%
72	Gly-Side-C3	Arg-Side-N2	0.02%
73	Gly-Side-C2	Arg-Side-N4	0.02%
74	Gly-Side-C2	Arg-Side-N3	0.02%