Supplementary Information

An Experimental-Theoretical Study for Aggregation Structure of Calix[6]arenes in Langmuir Films at the water/air interface†

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Table S1. Potential parameters for fluids

Parameters of SPC-FH water model			
Site	ε_{ii} *(x10^{-2} kcal/mol)*	σ_{ii} *(Å)*	q_i *(e)*
O	15.525	3.188	-0.8476
H	3.965	0.650	0.4238
	Intramolecular parameters		
	k_b *(kcal/mol/Å^2)*	k_θ *(kcal/mol/rad^2)*	θ-θ_0 *(°)*
O-H	553.92	45.74	109.4
Parameters of N_2 and O_2 gas			
Site	ε_{ii} *(x10^{-2} kcal/mol)*	σ_{ii} *(Å)*	q_i *(e)*
N	16.700	3.320	-
O	22.800	2.990	-

Table S2. Topology and Potential parameters for *Calix6* dimer by LAMMPS style and according to the *Calix6* model.

LAMMPS Calix 6 # units – real

156 atoms
162 bonds
294 angles

7 atom types
9 bond types
13 angle types

0.0000 40.0000 xlo xhi
0.0000 40.0000 ylo yhi
0.0000 40.0000 zlo zhi

Masses

1 12.011150
2 12.011150
3 15.999400
4 12.011150
5 12.011150
6 1.007970
7 1.007970

Pair Coeffs # pair style Lennard-Jones

1 0.14799 3.61704
2 0.03899 3.87540
3 0.22800 2.85978
4 0.15999 3.47450
5 0.03899 3.87540
6 0.03800 2.44997
7 0.03800 2.44997

Bond Coeffs # bond style Harmonic

1 384.0000 1.3700
2 480.0000 1.3400
3 283.0924 1.5100
4 363.4164 1.0800
5 283.0924 1.5100
6 340.6175 1.1050
7 540.6336 0.9600
8 322.7158 1.5260
9 340.6175 1.1050

Angle Coeffs # angle style Harmonic

1 60.0000 120.0000
2 90.0000 120.0000
3 44.2000 120.0000
4 37.0000 120.0000

5	44.2000	120.0000
6	44.4000	110.0000
7	46.6000	110.5000
8	39.5000	106.4000
9	50.0000	109.0000
10	46.6000	110.5000
11	46.6000	110.5000
12	44.4000	110.0000
13	39.5000	106.4000

Atoms # (atom, molecule, type, charge, x, y, z)

1	0	1	0.030000	-15.841334332	21.162318207	-17.359423749
2	0	1	0.000000	-15.841334332	21.162318207	-15.949423783
3	0	1	-0.100000	-14.619334329	21.162318207	-15.282423847
4	0	1	0.000000	-13.407334316	21.154318207	-15.970423691
5	0	1	-0.100000	-13.430334318	21.236318208	-17.359423749
6	0	1	0.000000	-14.628334273	21.224318206	-18.072423749
7	0	2	-0.200000	-17.110334385	21.185318207	-15.147423856
8	0	1	0.000000	-17.412334312	19.887318231	-14.458423726
9	0	1	-0.100000	-16.488334347	19.376318194	-13.549423806
10	0	1	0.000000	-16.723334361	18.200318314	-12.843423955
11	0	1	-0.100000	-17.950334299	17.561318137	-13.005423658
12	0	1	0.000000	-18.898334254	18.020318247	-13.915423744
13	0	1	0.030000	-18.614334334	19.181318261	-14.663423650
14	0	2	-0.200000	-20.186334122	17.262318112	-14.060423724
15	0	1	0.000000	-19.997334469	15.925318219	-14.714423768
16	0	1	-0.100000	-19.242334355	14.960318066	-14.052423827
17	0	1	0.000000	-18.999334324	13.707318284	-14.610423677
18	0	1	-0.100000	-19.611334313	13.385318257	-15.817423694
19	0	1	0.000000	-20.408334244	14.303318001	-16.501423769
20	0	1	0.030000	-20.565334309	15.595318295	-15.961423747
21	0	2	-0.200000	-21.110334385	13.872318245	-17.758423738
22	0	1	0.000000	-20.195334423	13.286318280	-18.789423697
23	0	1	-0.100000	-19.695334423	12.002318360	-18.578423731
24	0	1	0.000000	-18.802334297	11.410318352	-19.465423696
25	0	1	-0.100000	-18.488334406	12.082318284	-20.644423835
26	0	1	0.000000	-18.998334397	13.347318150	-20.921423785
27	0	1	0.030000	-19.828334320	13.969318368	-19.965423696
28	0	2	-0.200000	-18.672334421	13.989318348	-22.237423532
29	0	1	0.000000	-17.244334329	14.432318188	-22.349423520
30	0	1	-0.100000	-16.239334334	13.469318368	-22.352423780
31	0	1	0.000000	-14.894334305	13.809318043	-22.487423532
32	0	1	-0.100000	-14.561334360	15.145318009	-22.692423932
33	0	1	0.000000	-15.534334321	16.143318154	-22.706423871
34	0	1	0.030000	-16.880334366	15.785318352	-22.498423688
35	0	2	-0.200000	-15.120334316	17.557318188	-22.987423532
36	0	1	0.000000	-14.396334279	18.207318284	-21.846423738
37	0	1	0.030000	-14.897334326	19.345318176	-21.185423724
38	0	1	0.000000	-14.128334273	19.998318173	-20.201423757
39	0	1	-0.100000	-12.898334254	19.449318148	-19.846423738
40	0	1	0.000000	-12.417334307	18.282318093	-20.438423745
41	0	1	-0.100000	-13.159334410	17.696318127	-21.459423654
42	0	3	-0.380000	-16.135334332	19.783318259	-21.574423902
43	0	4	0.000000	-11.084334362	17.709318139	-19.997423761

44	0	5	-0.300000	-10.918334473	17.848318316	-18.481423728
45	0	2	-0.200000	-14.566334356	21.287318207	-19.568423860
46	0	4	0.000000	-13.838334311	12.722318627	-22.457423799
47	0	5	-0.300000	-12.458334435	13.290317990	-22.122423761
48	0	3	-0.380000	-17.893334378	16.704318024	-22.451423757
49	0	4	0.000000	-18.178334225	10.060317971	-19.176423781
50	0	5	-0.300000	-18.319334257	9.684318520	-17.700423740
51	0	3	-0.380000	-20.329334248	15.231317975	-20.127423637
52	0	4	0.000000	-18.030334223	12.765317894	-13.924423806
53	0	5	-0.300000	-18.178334225	11.327318169	-14.421423785
54	0	3	-0.380000	-21.284334172	16.582318284	-16.581423752
55	0	4	0.000000	-15.649334330	17.568318106	-11.981423967
56	0	5	-0.300000	-14.594334353	18.586318232	-11.546423547
57	0	3	-0.380000	-19.476334322	19.689318158	-15.596423738
58	0	4	0.000000	-12.108334292	21.054318204	-15.197423808
59	0	5	-0.300000	-10.937334526	20.701318212	-16.116423719
60	0	3	-0.380000	-16.990334380	21.120318208	-18.101423733
61	0	5	-0.300000	-9.976334561	18.491318203	-20.706423633
62	0	5	-0.300000	-10.964334477	16.227318265	-20.353423707
63	0	5	-0.300000	-13.793334234	12.070318200	-23.841423623
64	0	5	-0.300000	-14.188334335	11.666317917	-21.405423753
65	0	5	-0.300000	-18.888334263	9.007318474	-20.030423753
66	0	5	-0.300000	-16.689334322	10.088317849	-19.530423753
67	0	5	-0.300000	-18.256334294	12.783318497	-12.410423867
68	0	5	-0.300000	-16.611334313	13.261318184	-14.224423759
69	0	5	-0.300000	-16.266334344	16.939318158	-10.731423967
70	0	5	-0.300000	-14.978334356	16.472318150	-12.817423932
71	0	5	-0.300000	-11.831334103	22.403318264	-14.531423681
72	0	5	-0.300000	-12.230334271	19.965318181	-14.126423709
73	0	6	0.100000	-16.126334328	10.732317902	-18.841423743
74	0	6	0.100000	-17.926334370	8.679318406	-17.506423749
75	0	6	0.100000	-16.421334315	13.288318135	-15.304423682
76	0	6	0.100000	-17.378334273	10.688318230	-14.026423805
77	0	6	0.100000	-15.856334331	12.606318451	-13.769423835
78	0	6	0.100000	-14.503334273	16.894318081	-13.713423841
79	0	6	0.100000	-18.140334357	11.265317894	-15.528423779
80	0	6	0.100000	-17.788334358	10.389318444	-17.034423761
81	0	6	0.100000	-16.250334341	9.084318139	-19.482423656
82	0	6	0.100000	-14.184334386	19.152318217	-12.409423940
83	0	6	0.100000	-16.443334330	14.280318238	-13.830423705
84	0	6	0.100000	-16.514334310	10.485318162	-20.551423661
85	0	6	0.100000	-15.706334326	15.711317994	-13.154423826
86	0	6	0.100000	-19.377334345	9.706317879	-17.388423748
87	0	6	0.100000	-14.200334299	15.952318169	-12.242423646
88	0	6	0.100000	-19.136334408	10.891318299	-14.108423822
89	0	6	0.100000	-13.752334345	18.092318274	-11.044423692
90	0	6	0.100000	-13.515334357	10.802318551	-21.473423593
91	0	6	0.100000	-18.468334425	8.006318070	-19.863423698
92	0	6	0.100000	-17.500334371	12.184318520	-11.888423555
93	0	6	0.100000	-14.109334338	12.070318200	-20.387423866
94	0	6	0.100000	-12.409334410	13.657318093	-21.086423747
95	0	6	0.100000	-15.012334336	19.323318221	-10.848423593
96	0	6	0.100000	-15.516334344	16.387318112	-10.151423566
97	0	6	0.100000	-12.317334402	18.968318202	-14.579423778
98	0	6	0.100000	-11.676334370	12.530318238	-22.244423978

99	0	6	0.100000	-19.243334282	12.383317925	-12.145423524
100	0	6	0.100000	-15.227334309	11.292318322	-21.517423742
101	0	6	0.100000	-19.959334362	8.962318398	-19.795423858
102	0	6	0.100000	-19.989334095	11.453318574	-17.664423756
103	0	6	0.100000	-19.445334423	12.378317811	-16.246423714
104	0	6	0.100000	-18.798334349	15.187318303	-13.064423673
105	0	6	0.100000	-18.152334440	16.652317978	-12.406423681
106	0	6	0.100000	-11.352334488	19.957318164	-13.468423717
107	0	6	0.100000	-18.792334307	9.234317757	-21.100423686
108	0	6	0.100000	-17.788334358	11.602317788	-21.354423635
109	0	6	0.100000	-9.944334496	15.859318234	-20.178423755
110	0	6	0.100000	-18.201334227	13.814318158	-12.018423669
111	0	6	0.100000	-11.050334442	19.698318221	-16.568423741
112	0	6	0.100000	-9.985334385	20.718318202	-15.572423808
113	0	6	0.100000	-12.207334269	14.145318009	-22.773423784
114	0	6	0.100000	-11.648334492	15.609318234	-19.753423803
115	0	6	0.100000	-13.127334345	20.107318260	-13.490423791
116	0	6	0.100000	-17.070334304	16.233318306	-11.002423875
117	0	6	0.100000	-9.914334286	17.538318135	-18.163423769
118	0	6	0.100000	-11.646334160	17.229318120	-17.941423766
119	0	6	0.100000	-16.705334354	17.700318314	-10.073423974
120	0	6	0.100000	-16.502334345	12.403318383	-22.218423955
121	0	6	0.100000	-15.528334338	19.902318217	-13.391423814
122	0	6	0.100000	-14.768334378	11.642317750	-24.109423749
123	0	6	0.100000	-13.052334297	11.260317780	-23.878423803
124	0	6	0.100000	-11.214334477	16.042318322	-21.412423723
125	0	6	0.100000	-10.866334427	21.412318207	-16.955423735
126	0	6	0.100000	-14.592334378	21.126318209	-14.177423827
127	0	6	0.100000	-21.867334355	13.109317757	-17.477423750
128	0	6	0.100000	-20.622334469	17.104318120	-13.052423589
129	0	6	0.100000	-13.498334397	15.426318146	-22.827423684
130	0	6	0.100000	-11.069334496	18.893318154	-18.141423754
131	0	6	0.100000	-10.904334534	22.376318194	-13.944423787
132	0	6	0.100000	-18.873334397	13.255318142	-23.045423620
133	0	6	0.100000	-13.526334275	12.801318146	-24.615423791
134	0	6	0.100000	-12.765334357	16.794318177	-21.968423955
135	0	6	0.100000	-12.474334229	21.278318204	-17.913423769
136	0	6	0.100000	-21.698334206	14.708318211	-18.196423762
137	0	6	0.100000	-12.285334337	19.935318209	-19.062423699
138	0	6	0.100000	-20.937334526	17.874318100	-14.606423728
139	0	6	0.100000	-8.981334198	18.134318091	-20.410423867
140	0	6	0.100000	-17.025334347	21.975318231	-14.372423761
141	0	6	0.100000	-12.646334398	22.686318256	-13.852423780
142	0	6	0.100000	-19.369334448	14.833318211	-22.437423818
143	0	7	0.350000	-21.531334389	16.266318299	-17.447423749
144	0	6	0.100000	-11.730334271	23.201318242	-15.278423660
145	0	7	0.350000	-20.009334553	15.568318345	-20.962423675
146	0	7	0.350000	-20.224334229	19.099318244	-15.656423800
147	0	6	0.100000	-10.030334461	19.561318256	-20.467423789
148	0	6	0.100000	-17.960334290	21.503318198	-15.791423790
149	0	6	0.100000	-10.055334557	18.390318133	-21.796423547
150	0	6	0.100000	-14.450334299	17.561318137	-23.872423761
151	0	7	0.350000	-17.507334340	17.570318200	-22.565423600
152	0	7	0.350000	-17.728334296	21.100318208	-17.496423744
153	0	6	0.100000	-13.841334332	22.076318182	-19.862423770

154	0	6	0.100000	-16.004334334	18.159318186	-23.295423620
155	0	7	0.350000	-16.390334357	20.496318199	-20.994423740
156	0	6	0.100000	-15.541334320	21.628318198	-19.981423728

Bonds # (id, type, atom1, atom2)

1	1	1	60
2	2	1	6
3	2	1	2
4	3	2	7
5	2	2	3
6	4	3	126
7	2	3	4
8	2	4	5
9	5	4	58
10	4	5	135
11	2	5	6
12	3	6	45
13	6	7	140
14	3	8	7
15	6	7	148
16	2	8	13
17	2	8	9
18	2	9	10
19	4	9	121
20	2	10	11
21	5	10	55
22	4	11	105
23	2	11	12
24	2	12	13
25	3	12	14
26	1	13	57
27	3	15	14
28	6	14	138
29	6	14	128
30	2	15	16
31	2	15	20
32	2	16	17
33	4	16	104
34	5	17	52
35	2	17	18
36	4	18	103
37	2	18	19
38	2	19	20
39	3	19	21
40	1	20	54
41	3	22	21
42	6	21	127
43	6	21	136
44	2	22	23
45	2	22	27
46	4	23	102
47	2	23	24
48	2	24	25
82	4	41	134
83	7	42	155
84	8	43	61
85	8	43	62
86	8	43	44
87	9	44	130
88	9	44	118
89	9	44	117
90	6	45	156
91	6	45	153
92	8	46	47
93	8	46	64
94	8	46	63
95	9	47	94
96	9	47	98
97	9	47	113
98	7	48	151
99	8	49	65
100	8	49	66
101	8	49	50
102	9	50	86
103	9	50	74
104	9	50	80
105	7	51	145
106	8	52	68
107	8	52	53
108	8	52	67
109	9	53	79
110	9	53	88
111	9	53	76
112	7	54	143
113	8	55	69
114	8	55	56
115	8	55	70
116	9	56	95
117	9	56	89
118	9	56	82
119	7	57	146
120	8	58	72
121	8	58	71
122	8	58	59
123	9	59	111
124	9	59	125
125	9	59	112
126	7	60	152
127	9	61	139
128	9	61	147
129	9	61	149

49	5	24	49
50	2	25	26
51	4	25	108
52	3	26	28
53	2	26	27
54	1	27	51
55	6	28	142
56	3	29	28
57	6	28	132
58	2	29	34
59	2	29	30
60	4	30	120
61	2	30	31
62	5	31	46
63	2	31	32
64	4	32	129
65	2	32	33
66	3	33	35
67	2	33	34
68	1	34	48
69	6	35	150
70	6	35	154
71	3	36	35
72	2	36	37
73	2	36	41
74	1	37	42
75	2	37	38
76	2	38	39
77	3	38	45
78	2	39	40
79	4	39	137
80	5	40	43
81	2	40	41
130	9	62	109
131	9	62	114
132	9	62	124
133	9	63	123
134	9	63	122
135	9	63	133
136	9	64	100
137	9	64	90
138	9	64	93
139	9	65	101
140	9	65	91
141	9	65	107
142	9	66	81
143	9	66	84
144	9	66	73
145	9	67	99
146	9	67	110
147	9	67	92
148	9	68	75
149	9	68	83
150	9	68	77
151	9	69	116
152	9	69	119
153	9	69	96
154	9	70	78
155	9	70	87
156	9	70	85
157	9	71	131
158	9	71	141
159	9	71	144
160	9	72	97
161	9	72	106
162	9	72	115

Angles # (id, type, atom1, atom2, atom3)

1	1	6	1	60
2	1	2	1	60
3	2	6	1	2
4	3	1	2	7
5	2	1	2	3
6	3	3	2	7
7	4	2	3	126
8	2	2	3	4
9	4	4	3	126
10	2	3	4	5
11	5	3	4	58
12	5	5	4	58
13	4	4	5	135
14	2	4	5	6
15	4	6	5	135
16	2	1	6	5
17	3	1	6	45
18	3	5	6	45
19	6	2	7	140
148	12	43	44	117
149	13	130	44	118
150	13	130	44	117
151	13	118	44	117
152	7	6	45	38
153	6	6	45	156
154	6	6	45	153
155	6	38	45	156
156	6	38	45	153
157	8	156	45	153
158	10	31	46	47
159	10	31	46	64
160	10	31	46	63
161	11	47	46	64
162	11	47	46	63
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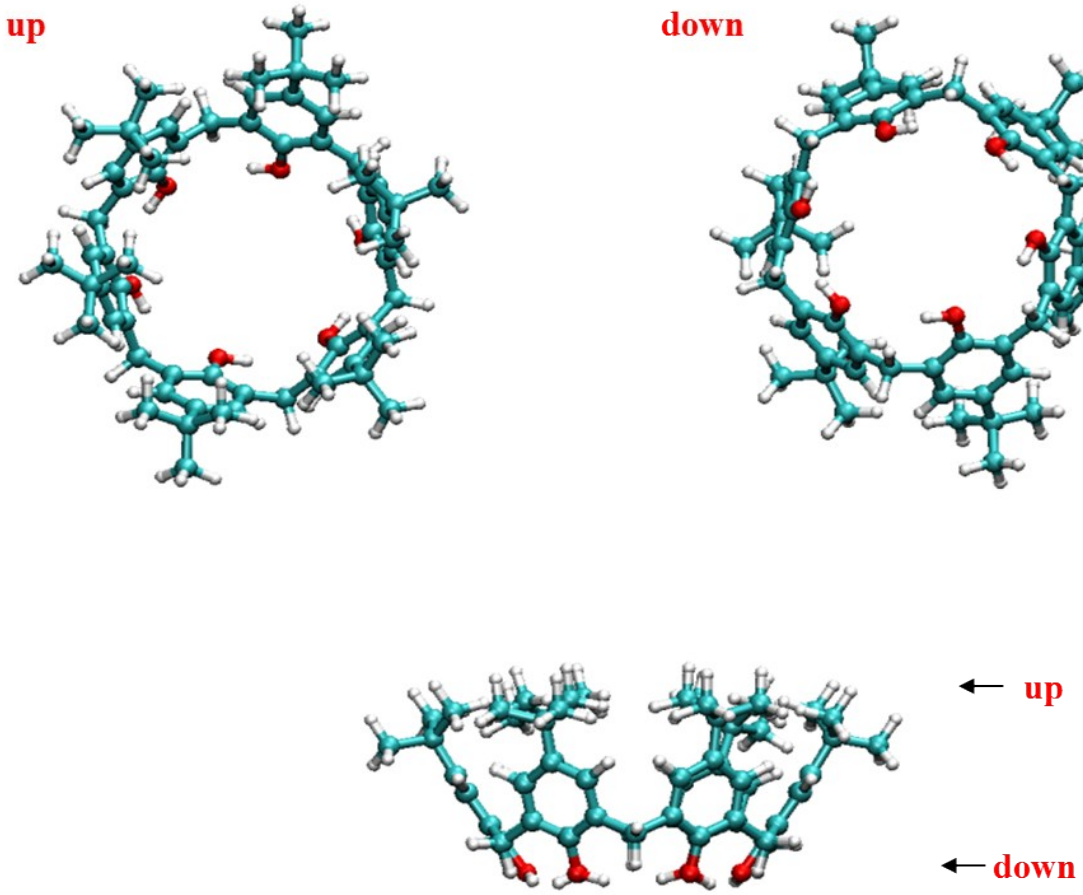
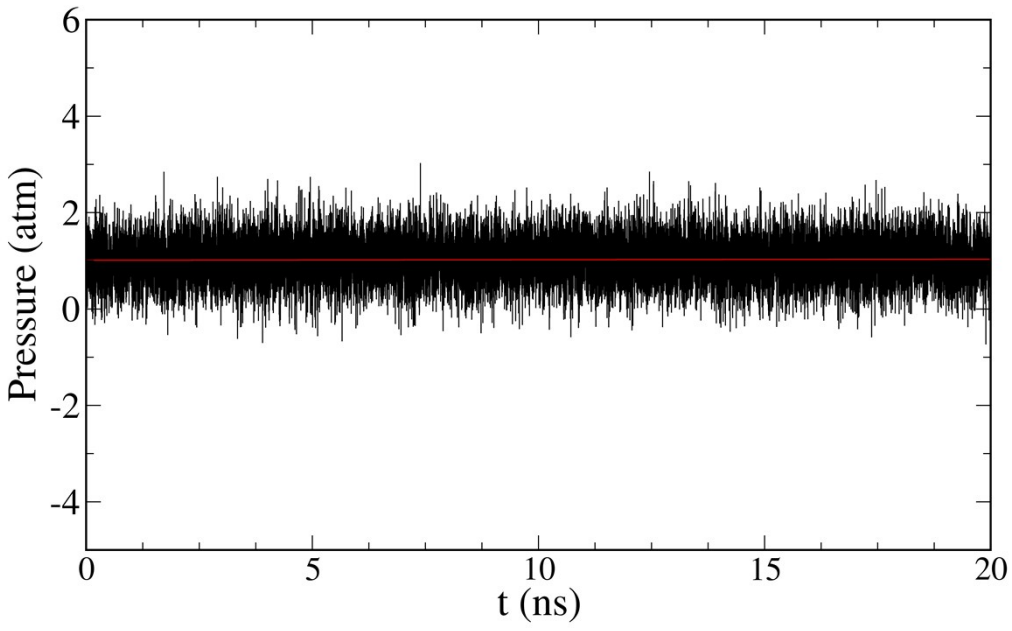


(a)



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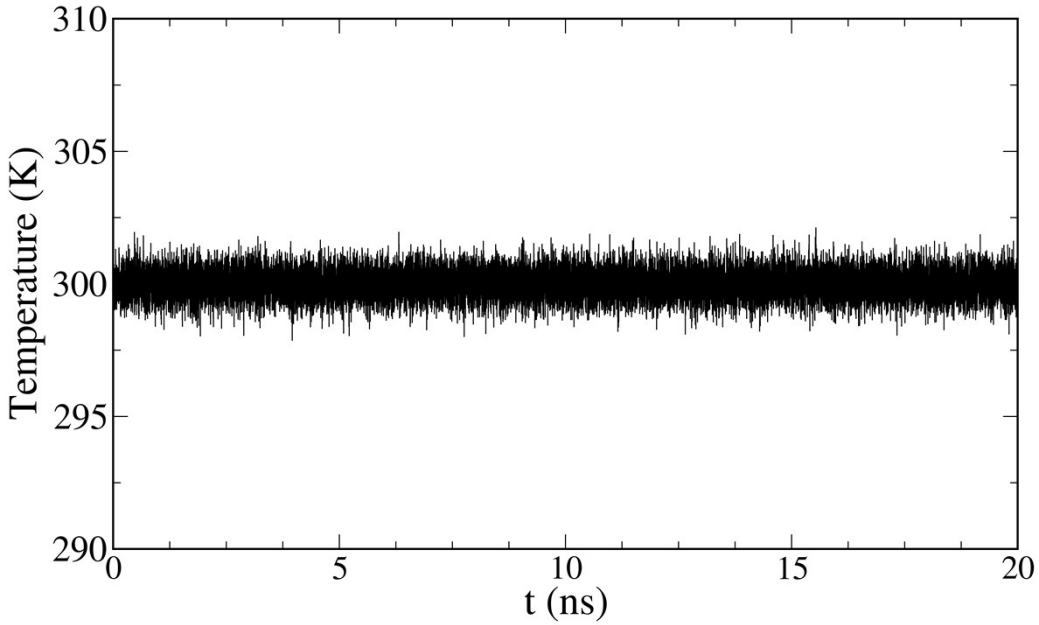

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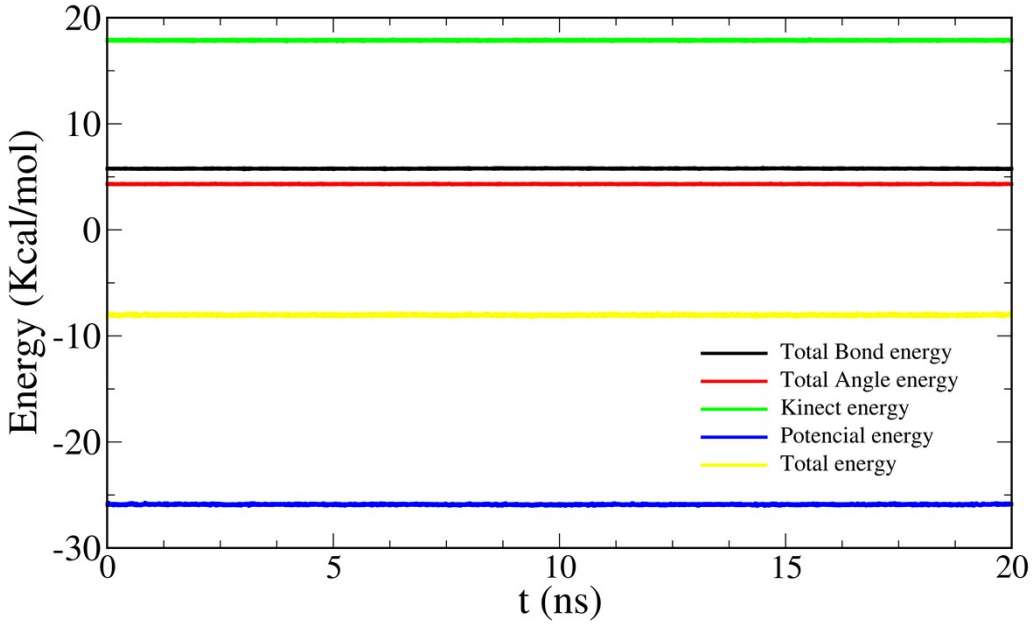

(d)

Figure S1. (a) Isolated *Calix6* molecule at up and down views; (b, c, d) Thermodynamic parameter equilibration by water/*Calix6* model.

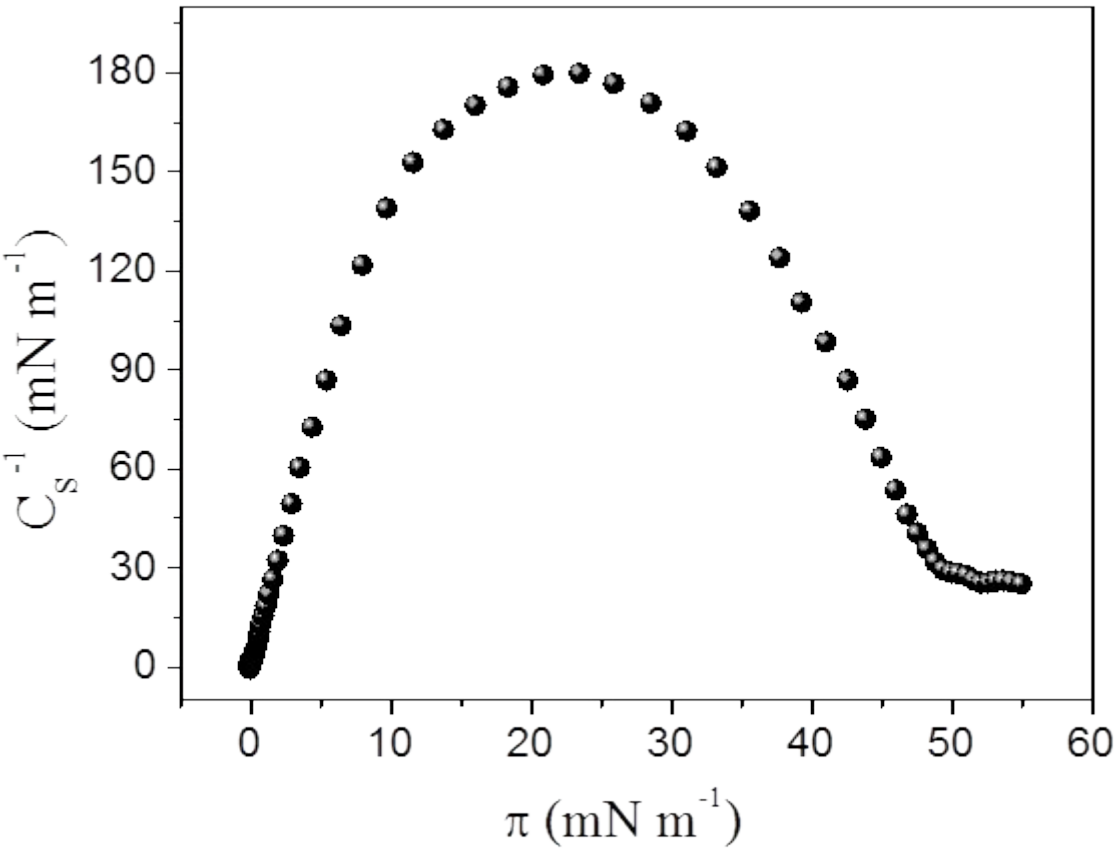

Figure S2. Compressibility modulus for *Calix6* monolayer at water/air interface.

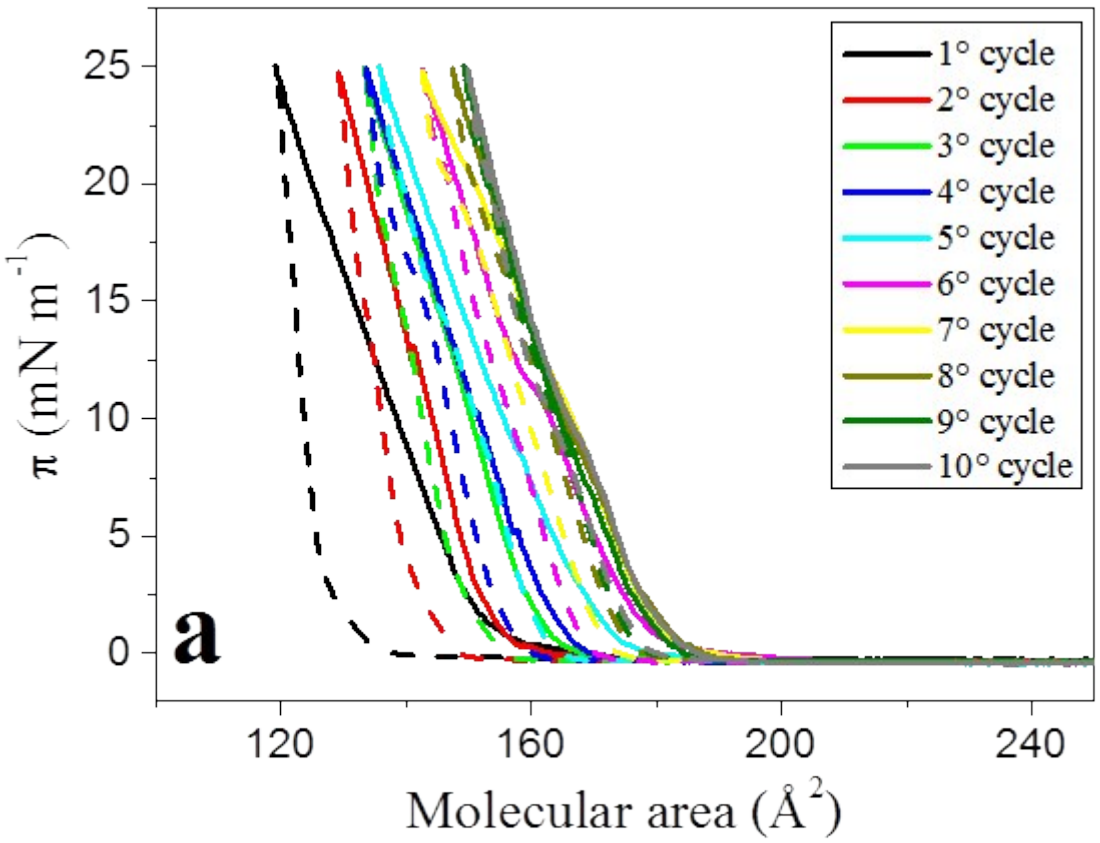

Figure S3. Compression–expansion cycles of *Calix6* monolayer on water subphase. Solid and dashed curves represent the compression and expansion cycles of the monolayer, respectively.

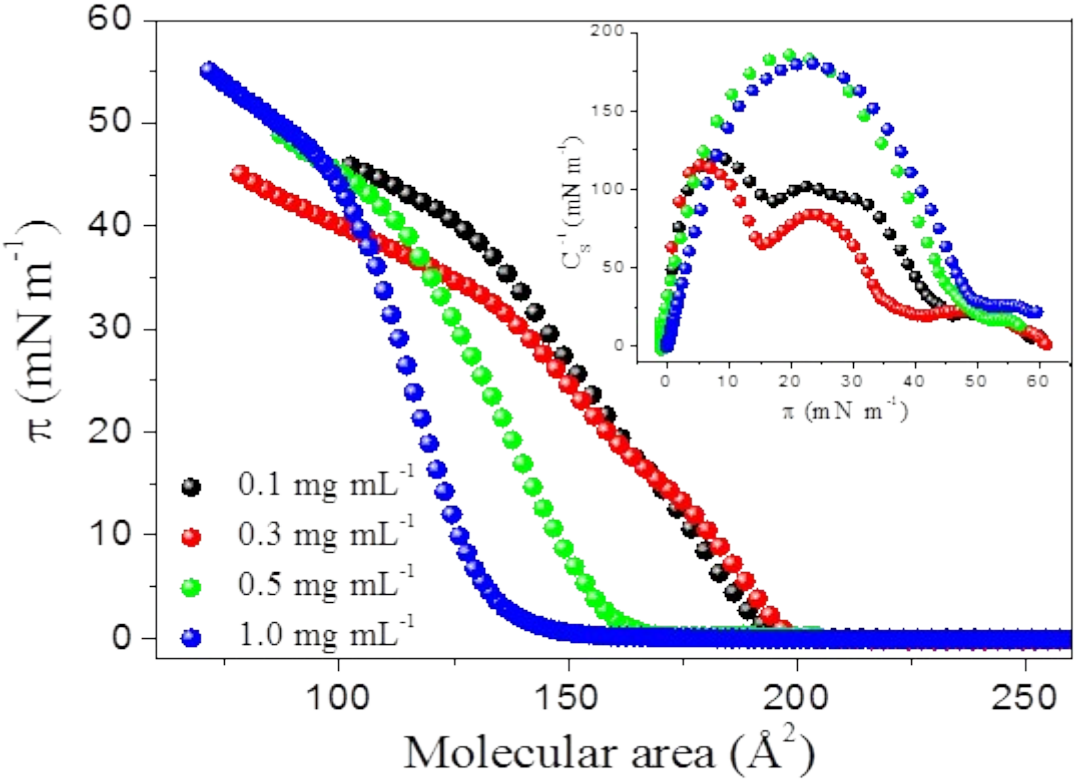

Figure S4. The effect of solution concentration on the *Calix6* monolayers.

By request of the referee, we have attached this data file generated by the simulation related to thermodynamic equilibration phase settings. This file is named as “output.dat”.


output.dat