

Coarse-Grained Molecular Dynamics Simulation of interface behaviour and self-assembly of CTAB
Cationic Surfactant: CTAB molecule in a water box

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1CTA	NC3	1	1.394	1.377	2.480
1CTA	C1	2	1.436	1.448	2.180
1CTA	C2	3	1.394	1.414	1.880
1CTA	C3	4	1.358	1.390	1.580
1CTA	C4	5	1.401	1.377	1.280
2W	W	6	1.693	1.847	1.568
3W	W	7	1.208	1.695	1.732
4W	W	8	0.523	1.163	3.484
5W	W	9	2.628	1.702	0.743
6W	W	10	0.564	0.928	2.959
7W	W	11	0.617	1.720	2.405
8W	W	12	2.041	1.846	2.027
9W	W	13	1.087	2.619	2.628
10W	W	14	0.446	2.147	2.199
11W	W	15	1.482	2.119	3.391
12W	W	16	1.710	1.675	2.449
13W	W	17	2.002	2.459	2.092
14W	W	18	2.059	2.268	3.428
15W	W	19	0.881	0.776	1.547
16W	W	20	1.094	0.730	2.851
17W	W	21	2.102	1.332	1.951
18W	W	22	2.475	0.868	1.383
19W	W	23	0.503	1.061	1.665
20W	W	24	1.667	2.351	1.651
21W	W	25	1.689	0.756	2.744
22W	W	26	1.137	2.390	0.509
23W	W	27	0.792	1.423	0.688
24W	W	28	2.243	1.363	1.128
25W	W	29	0.409	2.113	1.322
26W	W	30	1.520	2.528	2.895
27W	W	31	2.601	2.282	1.377
28W	W	32	0.944	1.702	2.851
29W	W	33	0.819	0.495	1.932
30W	W	34	2.587	0.842	2.493
31W	W	35	1.780	1.483	0.991
32W	W	36	1.349	0.767	3.655
33W	W	37	1.437	0.486	0.987
34W	W	38	0.815	2.472	2.169
35W	W	39	2.350	1.797	3.423
36W	W	40	2.517	0.407	2.175
37W	W	41	1.129	1.310	2.238
38W	W	42	0.683	2.510	3.012
39W	W	43	2.151	2.189	1.623
40W	W	44	2.369	1.421	2.403
41W	W	45	0.736	1.187	2.523
42W	W	46	0.474	1.466	2.852
43W	W	47	1.001	0.882	0.736
44W	W	48	1.991	1.109	1.448

45W	W	49	1.875	2.673	2.505
46W	W	50	1.339	0.899	1.400
47W	W	51	1.344	1.127	0.425
48W	W	52	2.145	1.736	2.819
49W	W	53	0.413	2.445	2.574
50W	W	54	2.117	2.263	0.732
51W	W	55	1.385	0.578	0.502
52W	W	56	1.608	1.215	2.369
53W	W	57	1.034	1.171	1.767
54W	W	58	1.187	2.698	0.927
55W	W	59	2.350	1.160	2.810
56W	W	60	2.593	2.218	0.859
57W	W	61	2.268	1.319	0.428
58W	W	62	1.107	2.136	3.661
59W	W	63	2.520	0.838	3.203
60W	W	64	1.715	0.606	1.484
61W	W	65	0.719	0.615	2.566
62W	W	66	0.767	1.578	1.936
63W	W	67	0.878	1.184	1.156
64W	W	68	1.137	0.833	2.276
65W	W	69	2.251	1.405	3.216
66W	W	70	0.399	1.095	0.694
67W	W	71	0.556	2.468	0.427
68W	W	72	0.812	2.046	3.184
69W	W	73	1.803	2.151	2.978
70W	W	74	1.888	0.518	0.670
71W	W	75	0.951	1.261	3.100
72W	W	76	2.252	0.516	3.464
73W	W	77	1.307	1.251	2.759
74W	W	78	1.277	0.599	1.869
75W	W	79	1.507	1.014	1.925
76W	W	80	0.664	2.000	0.645
77W	W	81	1.774	0.501	3.364
78W	W	82	1.871	1.794	3.267
79W	W	83	1.632	1.401	3.242
80W	W	84	2.669	1.734	2.895
81W	W	85	1.229	2.106	2.924
82W	W	86	0.894	0.778	3.334
83W	W	87	1.233	1.801	2.387
84W	W	88	1.602	1.615	0.509
85W	W	89	1.990	2.083	2.497
86W	W	90	0.948	1.924	1.383
87W	W	91	2.031	2.048	1.146
88W	W	92	0.992	2.052	2.062
89W	W	93	2.072	0.990	2.372
90W	W	94	1.762	0.891	1.042
91W	W	95	2.560	1.356	1.605
92W	W	96	1.361	1.151	0.899
93W	W	97	1.521	1.993	2.060
94W	W	98	0.784	2.480	3.522
95W	W	99	1.215	2.391	1.452

96W	W 100	1.964	0.817	1.888
97W	W 101	2.094	1.752	0.688
98W	W 102	0.740	2.301	1.707
99W	W 103	2.030	0.943	3.171
100W	W 104	2.543	1.892	1.847
101W	W 105	2.310	0.504	1.737
102W	W 106	1.868	1.229	2.799
103W	W 107	1.568	0.598	2.268
104W	W 108	0.799	2.402	1.109
105W	W 109	0.684	0.945	2.108
106W	W 110	0.484	0.764	1.185
107W	W 111	0.608	1.667	1.212
108W	W 112	1.299	1.656	0.937
109W	W 113	1.405	2.264	2.463
110W	W 114	2.289	0.797	0.799
111W	W 115	1.658	2.060	0.684
112W	W 116	1.541	1.727	2.913
113W	W 117	0.577	1.643	3.344
114W	W 118	2.337	2.120	3.070
115W	W 119	0.841	2.175	2.617
116W	W 120	1.142	1.910	0.484
117WF	WF 121	1.285	0.443	3.286
118WF	WF 122	2.590	1.176	0.834
119WF	WF 123	2.152	2.535	2.958
120WF	WF 124	2.105	0.536	2.546
121WF	WF 125	1.507	2.122	1.145
122WF	WF 126	2.123	1.659	1.553
123WF	WF 127	2.494	0.951	1.941
124WF	WF 128	0.535	0.638	0.671
125WF	WF 129	1.696	2.612	0.761
126WF	WF 130	1.626	1.532	1.943
127WF	WF 131	1.161	1.737	3.318
128WF	WF 132	1.813	1.108	0.602
129WF	WF 133	2.110	0.473	1.210
130ION	CL- 134	1.456	0.889	3.161
3.00000	3.00000	4.00000		