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Supporting Information

Machine-Learning-Assisted Screening of Pure-Silica Zeolites for Effective

Removal of Linear Siloxanes and Derivatives

Shiru Lin,[†] Yekun Wang,[‡] Yinghe Zhao,[†] Luis R. Pericchi[‡],

Arturo J. Hernández-Maldonado^{§,*} Zhongfang Chen^{†,*}

[†] Department of Chemistry, University of Puerto Rico, Rio Piedras, San Juan, PR 00931, USA

[‡] Department of Mathematics, University of Puerto Rico, Rio Piedras, San Juan, PR 00931, USA

[§] Department of Chemical Engineering, University of Puerto Rico, Mayagüez Campus, Mayagüez, PR 00681, USA

* To whom correspondence should be addressed. Email: zhongfangchen@gmail.com

(Z.C.)

Table S1. The identification numbers of the 500 randomly selected pure silica zeolites, and the average adsorption loading (L/mol), and adsorption energy (E/kcal/mol) towards DMSO₂, TMS, DMSD, MMST by GCMC simulations.

Num.	<i>L</i> for DMSO _z	<i>E</i> for DMSO ₂	<i>L</i> for TMS	<i>E</i> for TMS	<i>L</i> for DMSD	<i>E</i> for DMSD	<i>L</i> for MMST	<i>E</i> for MMST
110	12.0	21.20	8.0	18.41	9.4	17.93	11.9	17.18
216	11.7	21.58	6.5	18.56	9.8	17.91	11.8	17.14
305	12.0	21.40	8.0	18.98	8.9	17.79	11.9	16.97
416	11.0	21.21	6.5	19.35	10.2	18.37	11.0	16.57
726	11.8	21.48	7.1	19.27	9.0	18.29	10.9	17.00
729	11.0	21.40	7.8	19.48	9.8	18.38	10.6	17.03
863	11.2	21.76	5.0	17.28	8.8	17.08	11.8	17.20
877	11.7	21.67	7.9	18.16	9.7	17.82	11.5	17.10
908	10.9	21.22	6.0	17.73	8.1	17.94	11.8	17.79
959	11.0	21.37	7.5	19.13	8.6	18.27	10.4	16.88
972	10.0	21.00	8.0	18.99	9.1	18.31	11.9	18.02
1161	11.3	21.40	6.2	18.14	9.5	18.24	11.7	17.68
1197	10.8	21.74	3.6	16.78	6.0	18.33	10.7	16.34
1228	10.8	21.69	6.5	17.81	7.8	17.44	10.6	17.56
1365	10.3	21.52	6.7	18.22	8.0	17.59	9.6	17.52
1578	12.0	21.04	7.7	19.05	10.0	18.06	11.9	17.14
1579	13.0	21.01	7.7	19.37	10.7	17.91	13.0	17.72
1709	11.6	21.60	6.5	18.20	8.8	17.29	11.0	17.52
1827	12.0	21.37	8.9	19.81	9.6	18.60	11.8	17.52
1914	11.9	21.62	7.3	19.18	9.3	18.50	10.6	17.03
1932	12.0	21.70	6.5	17.43	8.6	16.58	12.0	17.89
2123	10.4	21.68	5.9	18.07	9.1	17.90	10.5	17.55
2173	12.3	21.88	5.8	18.55	7.7	17.66	12.7	17.45
2244	12.8	22.22	3.3	16.74	5.8	16.72	12.8	16.13
2431	10.8	21.62	6.2	18.15	7.8	17.75	10.6	16.44
2469	11.0	21.26	7.8	19.08	8.8	18.00	11.7	18.10
2632	11.5	21.22	7.2	19.07	8.9	18.09	11.0	16.71
2782	12.0	21.30	6.9	19.01	9.7	18.27	12.3	17.74
2887	12.6	21.87	6.0	18.96	8.5	17.48	12.6	17.06
3081	12.0	22.04	4.8	17.20	8.2	16.34	11.5	16.68
3205	11.0	21.84	6.1	18.47	8.4	18.17	10.9	16.97
3214	12.0	21.97	4.8	17.66	7.2	17.97	11.7	16.82
3274	11.0	21.63	5.8	18.06	70.7	17.22	10.9	17.07
3275	11.0	21.64	5.9	18.36	7.8	18.09	10.0	17.41
3825	11.8	21.65	6.0	18.35	8.8	18.11	10.4	17.38

3845	12.8	22.13	5.4	18.36	6.2	17.86	13.3	16.07
3921	11.9	21.85	4.9	17.77	8.7	16.82	11.0	17.65
3983	11.0	21.78	6.6	18.70	8.1	18.16	10.9	16.63
4012	11.9	21.72	6.8	18.22	8.4	17.58	12.0	17.22
4130	12.4	21.93	6.5	17.58	9.9	17.05	10.4	17.52
4138	12.9	21.72	7.9	19.48	9.9	18.97	8.8	18.11
4539	11.8	21.50	8.0	19.73	9.4	18.39	11.9	17.45
4735	12.0	21.21	6.9	19.37	8.6	17.36	11.8	16.71
4861	12.3	20.57	8.0	19.70	8.8	17.87	11.7	16.26
4946	13.4	21.99	5.0	18.63	8.1	16.42	13.2	16.38
5060	12.0	21.21	6.9	18.05	9.9	18.38	12.0	16.82
5155	13.0	21.90	5.6	18.05	8.6	17.48	12.3	17.09
5179	11.6	21.22	7.8	19.75	8.0	18.04	11.0	16.72
5185	12.5	21.49	7.0	18.70	9.8	18.25	12.7	17.55
5206	11.0	21.39	5.6	17.10	8.3	17.34	10.9	16.82
5219	12.0	21.55	6.0	18.15	8.4	17.62	10.8	16.69
5321	12.0	21.24	7.9	19.47	9.5	17.65	11.9	16.87
5386	11.8	21.39	8.0	19.86	10.0	18.19	11.9	17.10
5457	13.7	21.33	7.0	18.95	10.0	17.08	12.8	17.18
5506	11.8	21.64	6.9	19.14	8.8	18.02	11.7	16.95
5631	12.7	21.10	8.0	19.60	11.9	18.39	13.0	17.22
5681	12.9	21.25	7.7	19.28	9.6	17.44	12.7	17.07
5762	12.1	21.47	7.0	19.31	8.6	17.99	12.0	16.99
5849	11.3	21.52	6.6	18.33	8.3	17.48	10.7	16.61
5985	12.6	21.49	6.9	18.92	7.4	17.59	11.8	16.29
6010	12.0	21.31	6.6	18.88	8.1	17.81	10.8	16.57
6018	12.0	21.40	6.5	18.93	9.0	17.53	11.9	17.19
6026	12.8	21.22	6.5	18.40	8.8	17.53	12.8	17.15
6030	11.9	21.78	7.8	18.89	7.8	17.94	11.7	16.48
6046	13.2	22.02	5.2	18.03	7.6	17.24	12.9	16.34
6059	12.1	21.42	7.0	18.96	8.0	17.19	12.0	17.04
6086	11.0	21.32	6.4	18.46	8.7	17.63	10.6	16.96
6107	10.9	21.30	6.0	18.43	8.8	17.76	11.1	16.61
6219	12.0	21.42	7.4	19.15	9.7	18.31	12.0	17.33
6333	12.0	20.93	8.8	20.03	11.4	18.69	12.8	17.18
6348	12.5	21.61	7.9	19.80	10.6	18.30	12.5	17.27
6434	11.6	21.42	7.0	19.51	9.8	18.13	11.9	16.61
6533	12.0	21.17	6.9	19.82	8.9	17.13	11.5	17.31
6593	11.5	21.63	6.7	19.37	9.3	18.05	12.0	16.83
6831	13.0	21.15	9.0	20.07	9.7	18.40	12.7	17.39
6849	11.0	21.03	8.0	19.50	10.1	17.76	11.2	16.62
6913	12.1	22.05	4.5	16.86	6.2	17.35	11.3	16.95
6923	10.5	21.68	6.0	17.17	6.4	17.13	10.6	17.35

6945	12.3	21.73	6.3	18.73	7.4	17.87	12.3	17.72
7176	12.3	21.81	6.4	18.42	8.9	17.81	11.9	17.18
7546	12.5	21.56	7.7	19.24	9.0	18.08	12.0	17.42
7649	11.8	21.31	7.9	19.20	9.0	17.89	11.9	17.16
7853	13.8	21.64	6.8	18.90	8.8	18.10	10.9	17.29
7959	11.6	21.94	5.9	18.18	7.8	17.33	10.7	16.78
7972	10.0	20.91	6.2	17.35	8.4	17.33	9.9	17.91
8156	12.7	21.53	6.9	19.01	7.8	17.69	11.9	16.62
8167	11.4	21.87	5.2	16.50	6.0	17.25	10.6	16.67
8234	10.1	21.58	4.6	17.44	6.4	17.59	1.7	16.65
8289	12.5	22.07	4.8	18.81	7.0	17.97	11.6	16.27
8305	12.8	21.80	6.0	18.98	8.1	17.16	13.4	16.49
8463	13.1	22.29	2.1	17.14	3.9	16.61	13.7	15.72
8470	13.1	22.22	5.4	18.53	5.8	17.83	12.0	16.29
8480	12.0	21.88	5.5	18.94	6.9	18.06	11.2	16.56
8561	12.3	21.72	6.0	18.69	8.2	17.70	11.7	16.37
8627	12.1	21.59	6.8	18.74	8.5	17.84	11.5	17.55
8675	11.3	21.98	2.9	17.19	5.6	17.22	10.7	16.29
8786	12.9	21.89	6.0	18.09	7.6	17.44	12.3	17.36
9209	11.3	21.61	7.9	19.24	8.6	18.27	9.9	16.94
9232	10.9	21.83	5.7	17.47	8.1	18.19	10.0	17.33
9270	10.6	21.45	7.5	18.99	8.5	18.31	10.9	17.11
9322	10.9	21.71	5.3	18.39	8.5	17.09	10.6	16.29
9439	11.7	21.62	7.3	18.79	8.9	18.18	10.9	16.70
9502	11.8	21.44	8.4	19.94	9.0	18.15	12.0	17.70
9596	12.4	21.53	7.0	18.94	8.7	17.89	10.7	16.95
9641	12.2	21.78	7.0	19.09	8.0	17.79	11.3	17.64
9643	12.8	21.69	8.0	19.80	9.3	18.34	11.9	17.41
9775	9.8	21.39	7.0	18.24	7.2	17.72	10.3	17.14
9894	12.6	21.93	5.7	18.19	8.4	18.17	12.8	17.61
9907	11.0	21.87	4.6	16.73	7.2	16.32	11.2	17.00
10050	11.0	21.81	5.0	17.79	8.6	17.24	10.8	17.24
10054	10.8	21.66	6.0	18.57	7.9	17.99	11.6	17.68
10072	10.4	21.27	7.1	18.54	9.9	17.97	10.9	17.25
10119	9.7	21.42	6.8	18.09	8.2	17.65	9.9	16.92
10389	9.9	21.45	6.9	18.17	8.8	17.69	9.6	17.07
10487	9.8	21.44	6.8	18.61	8.0	17.98	11.1	17.17
10772	11.4	21.58	6.7	19.14	8.3	17.54	12.4	17.25
10811	12.0	20.77	8.7	19.89	10.6	18.15	12.8	16.79
10867	12.1	21.64	5.7	18.57	9.1	17.30	12.2	16.81
10961	11.0	21.38	7.0	18.68	9.7	18.06	10.8	17.27
10995	11.7	21.32	8.8	19.21	9.4	18.10	11.0	16.45
11033	11.0	20.91	8.7	19.81	9.7	18.24	11.9	17.72

11040	10.8	20.87	9.0	19.88	9.7	18.15	11.7	17.83
11108	12.3	21.70	6.8	19.54	7.6	17.93	12.4	17.16
11140	11.0	20.96	8.9	19.46	9.3	18.27	11.2	17.51
11364	10.9	21.85	7.4	18.24	8.0	18.26	10.5	17.80
11487	11.6	21.85	6.8	18.90	7.7	18.02	11.1	17.11
11718	12.8	21.11	8.9	20.34	9.9	18.30	11.3	17.06
11852	12.0	21.75	7.5	19.19	9.0	18.14	12.0	17.73
11960	11.8	21.53	7.7	19.27	8.3	18.35	11.4	16.69
11962	12.8	21.16	8.0	19.45	8.8	17.91	12.4	17.55
12005	11.6	21.63	6.8	18.75	7.9	17.83	10.5	16.58
12061	9.7	20.96	8.3	19.99	9.0	18.67	9.7	16.84
12251	11.0	21.49	5.9	17.47	8.3	17.75	11.0	17.41
12385	12.0	21.74	7.6	18.99	9.2	18.21	11.6	16.97
12641	11.0	21.41	8.4	19.03	10.0	18.24	11.0	17.29
12791	11.8	21.30	8.0	19.93	9.1	19.05	11.9	16.71
12931	11.0	21.37	7.6	19.18	8.8	18.16	11.0	16.99
12975	11.5	22.01	4.7	18.31	6.0	18.41	10.9	15.98
13048	11.6	21.53	7.3	19.46	8.0	18.46	11.6	16.61
13436	11.8	21.79	8.0	19.83	8.9	18.17	11.9	17.00
13440	10.9	21.01	7.9	19.74	9.7	18.51	11.7	17.53
13535	11.4	21.68	8.0	19.61	9.8	18.06	11.3	17.28
13640	10.6	21.42	8.7	19.96	8.9	18.82	10.5	17.13
13771	11.9	21.48	9.0	19.92	10.0	18.94	11.7	17.18
13848	12.7	21.11	8.0	19.49	10.6	18.71	12.9	17.14
13871	10.7	21.47	7.7	18.63	8.0	17.89	11.1	17.40
13887	12.0	21.43	8.8	20.10	9.6	18.48	10.8	17.35
13981	12.0	20.99	9.0	20.35	9.0	18.27	11.0	17.04
14197	12.9	21.09	7.9	19.16	9.2	18.01	11.9	17.54
14236	10.5	21.54	5.3	17.58	8.8	17.56	10.2	17.83
14309	11.0	21.46	5.1	17.63	8.8	17.62	10.6	16.69
14481	11.8	21.83	5.8	17.61	6.6	17.61	11.8	16.50
14738	12.0	21.40	6.9	18.52	8.3	18.15	11.3	17.22
14813	11.9	21.55	6.0	17.88	7.4	16.61	12.3	16.60
14890	11.0	21.16	7.9	19.31	9.4	18.59	10.0	17.23
14908	11.0	21.49	6.7	18.41	10.0	18.17	11.0	16.89
15047	9.8	21.42	6.3	18.47	9.0	17.53	9.1	16.66
15169	11.7	21.87	4.5	17.73	8.5	17.61	11.9	17.03
15317	10.2	21.20	6.2	18.78	9.7	18.42	10.6	18.00
15327	12.0	21.41	6.9	18.52	9.6	18.33	12.9	18.03
15359	10.9	21.56	6.8	18.82	8.0	18.16	8.2	18.19
15377	9.8	21.42	6.6	18.56	8.9	18.04	10.5	17.63
15393	12.6	22.02	4.8	18.20	6.2	17.69	11.4	16.22
15504	11.9	21.73	6.7	18.76	7.0	17.98	12.2	17.15

15972	10.5	21.54	6.5	18.41	7.9	17.91	10.2	16.95
15980	9.7	21.54	4.8	17.14	7.3	17.56	10.0	16.99
16108	9.4	21.63	3.4	15.17	5.9	16.82	9.1	16.99
16119	10.9	21.37	4.9	16.29	7.1	17.43	11.3	17.34
16121	10.1	21.32	4.5	16.37	6.8	17.46	9.7	17.60
16196	8.5	21.51	2.8	15.73	6.0	16.68	8.1	17.01
16501	10.9	21.74	5.5	17.00	7.6	17.42	10.2	18.40
16671	9.8	21.41	6.1	17.42	7.9	17.66	10.6	17.72
16893	10.0	21.68	4.5	16.75	7.7	17.99	10.8	17.33
16961	10.6	21.36	6.2	18.38	8.4	18.08	11.5	17.20
17033	9.7	21.91	3.7	15.85	6.0	17.23	9.7	16.92
17229	11.0	21.45	7.0	18.28	8.2	17.86	11.8	18.24
17360	11.8	21.68	7.4	18.81	8.0	18.46	11.0	18.10
17527	10.8	21.78	5.6	17.68	8.8	17.69	10.5	17.64
17629	11.9	21.69	4.3	17.30	6.1	17.47	11.0	16.75
17840	13.7	21.49	8.0	19.09	8.0	17.45	11.6	16.95
17905	10.6	21.39	6.0	18.53	8.2	18.38	10.9	16.59
17965	10.1	21.55	3.9	17.05	5.4	17.00	10.3	16.91
18082	9.5	21.76	2.9	15.69	6.0	17.00	9.8	16.87
18276	9.8	21.34	5.3	16.98	5.7	17.22	9.9	16.91
18294	10.8	21.85	5.1	16.58	6.8	17.98	8.2	16.88
18647	10.0	21.53	6.6	17.92	8.5	17.80	10.0	17.48
18726	9.8	21.74	5.8	17.88	7.9	18.74	8.8	16.98
18749	11.3	21.61	7.0	17.83	8.7	17.96	11.1	17.44
18886	10.9	21.83	5.4	17.55	8.5	18.14	9.8	17.45
18940	8.3	21.29	4.4	16.17	6.9	17.20	7.9	16.36
18941	10.6	21.81	4.9	16.63	6.3	16.86	9.6	16.24
18969	9.6	21.80	3.3	15.90	6.6	17.11	9.6	18.40
19261	11.1	21.89	5.1	18.13	6.8	18.11	11.7	16.42
19270	10.4	21.62	5.7	18.01	7.7	17.97	10.7	16.60
19283	10.2	21.38	5.7	19.38	8.8	17.86	10.0	17.03
19328	10.0	21.38	6.9	18.97	7.8	18.52	9.8	16.59
19330	11.2	21.80	5.3	17.87	7.6	17.25	9.5	17.13
19416	10.8	21.73	5.2	17.48	6.8	17.32	10.4	17.26
19660	11.8	21.77	6.0	17.84	9.9	18.14	11.8	17.70
19732	11.4	21.72	5.4	18.01	8.2	17.42	11.0	17.75
19846	11.6	21.79	4.9	17.61	6.9	17.41	11.0	17.46
19853	13.0	21.79	7.4	18.98	8.2	18.17	12.8	17.73
19959	10.9	21.79	6.2	17.39	7.5	17.44	11.0	17.83
19969	11.0	21.63	5.5	17.83	7.0	17.89	11.1	17.62
20023	10.0	21.81	3.7	16.23	7.2	17.60	9.7	16.96
20085	9.6	21.66	5.6	16.80	8.6	16.89	9.7	17.55
20167	11.0	21.63	5.3	17.55	8.1	17.66	10.1	17.18

20374	11.6	21.89	5.7	17.77	6.4	17.52	8.8	16.16
20387	10.0	21.84	2.4	16.33	6.9	17.17	9.7	16.24
20536	10.8	21.84	6.6	18.32	8.9	18.14	10.0	17.78
20631	9.9	21.61	4.9	16.71	7.3	17.49	8.9	16.95
20645	9.6	21.58	4.4	16.56	8.0	17.57	9.2	16.51
20650	10.5	21.76	4.0	17.10	7.9	17.71	10.1	17.45
20684	10.8	21.82	3.8	16.07	6.0	17.69	10.6	16.67
20844	10.1	21.62	3.3	16.08	6.0	18.14	9.7	16.11
20880	10.4	21.62	6.5	18.30	8.4	17.76	10.4	17.89
20926	10.5	21.85	3.4	15.84	4.9	17.14	11.2	16.07
21006	10.9	21.58	6.6	17.93	8.0	18.23	10.6	17.47
21080	10.1	21.66	6.0	18.25	9.9	18.22	10.0	17.42
21522	10.8	21.89	5.5	17.47	7.5	17.72	10.3	16.84
21772	11.7	21.93	5.6	18.29	7.7	17.18	11.7	17.04
21938	9.6	21.45	6.3	18.64	7.0	18.17	10.5	17.04
21959	11.9	22.01	6.8	18.79	7.6	18.12	10.9	17.44
22163	12.0	21.58	6.2	18.19	7.9	17.75	10.8	16.67
22233	11.0	22.06	4.1	17.26	7.8	17.51	11.0	17.12
22251	10.4	21.85	4.5	16.99	6.2	17.14	10.7	16.74
22301	9.6	21.64	2.8	17.11	6.0	17.51	8.8	15.91
22323	10.7	21.79	4.2	16.53	6.8	17.28	10.6	18.28
22424	10.8	21.73	6.5	18.24	7.0	17.83	11.3	17.62
22447	11.9	22.10	3.4	16.05	5.9	16.90	11.3	16.75
22555	10.9	21.98	3.7	16.76	5.9	17.10	8.8	16.66
22598	9.0	21.51	3.9	15.53	7.3	17.01	8.7	16.95
22712	9.0	21.47	6.5	17.88	7.4	17.81	10.4	17.35
22856	11.8	21.75	6.7	18.32	8.2	17.11	10.6	16.96
22858	12.7	21.58	6.9	18.71	9.5	18.00	11.9	17.20
23079	12.7	21.99	6.0	18.24	7.9	17.68	11.7	16.85
23305	11.0	21.87	5.4	17.43	8.4	17.46	11.0	17.50
23398	10.0	21.21	7.9	19.23	8.7	18.20	10.2	17.07
23416	11.1	21.79	6.0	18.57	7.5	17.74	9.8	16.66
23565	10.3	21.59	6.8	18.47	7.8	18.19	11.0	17.30
23650	11.4	21.55	7.5	19.30	8.4	18.18	10.7	17.30
23692	11.0	21.46	7.8	19.20	8.5	18.13	10.6	17.05
23699	9.9	21.02	7.9	19.23	8.3	18.26	9.9	16.60
23768	10.1	21.46	5.8	17.51	8.4	18.00	10.4	17.35
23774	10.8	21.71	6.4	18.49	8.0	17.95	10.4	17.81
23983	13.3	21.18	7.0	18.96	9.0	17.68	11.9	17.70
24078	12.4	21.84	6.0	18.01	9.1	17.92	12.1	17.55
24196	12.0	21.88	6.3	18.41	9.2	17.75	11.4	17.62
24299	10.7	21.10	6.2	19.05	8.4	17.25	11.0	16.67
24434	12.0	21.47	7.9	19.88	9.3	18.19	11.6	17.39

24468	11.6	21.35	7.7	19.38	8.1	18.17	10.9	17.54
24489	11.9	21.91	5.5	18.14	7.2	17.63	11.8	16.65
24493	11.6	21.65	6.6	19.04	9.0	18.55	11.4	17.53
24553	11.9	21.37	9.0	20.36	9.0	18.63	11.7	17.33
24601	11.4	21.71	7.3	18.66	8.7	18.00	11.1	17.76
24746	12.7	21.22	7.0	19.04	9.6	17.94	12.4	17.33
24839	11.8	21.91	5.0	17.68	7.8	17.96	11.2	16.67
24929	11.5	21.76	5.6	18.21	8.0	17.90	11.5	16.37
25000	10.0	21.21	7.9	19.68	9.4	18.55	10.1	16.86
25194	13.0	21.98	6.9	18.40	8.5	18.06	11.6	16.97
25535	10.8	21.07	8.5	19.53	9.9	18.64	9.9	16.64
25537	11.7	21.89	6.0	17.68	7.8	17.79	11.6	17.60
25604	10.9	21.73	6.3	17.89	8.8	17.75	10.5	17.54
25639	11.9	21.86	7.3	18.72	10.6	18.30	11.0	16.89
25676	12.9	22.20	5.0	18.23	7.1	17.79	11.3	16.61
25690	11.8	21.78	6.4	18.82	8.7	18.27	11.8	17.36
25819	10.4	21.53	6.0	18.26	6.7	17.88	9.6	16.76
25821	11.0	21.53	6.8	18.76	10.2	18.10	11.0	17.23
25913	12.1	21.82	5.7	18.22	6.3	17.86	11.8	18.05
25919	11.9	21.70	5.8	18.51	9.3	17.08	12.0	16.69
25920	11.9	22.04	4.4	17.67	6.8	17.66	10.7	16.89
25925	10.8	21.73	5.0	17.82	6.4	18.21	10.2	16.41
26054	11.8	21.56	7.5	19.30	9.1	18.55	11.0	17.30
26078	10.8	21.58	5.9	19.01	9.0	18.41	11.0	16.66
26083	12.2	21.92	4.8	18.14	7.4	16.85	11.0	16.43
26158	11.0	21.68	6.7	18.93	8.1	18.24	10.8	16.66
26167	12.7	21.41	7.5	19.65	9.6	18.48	12.1	17.14
26200	10.8	21.12	9.2	19.88	10.5	18.46	12.0	16.77
26405	10.9	21.59	8.8	20.18	9.0	19.05	10.9	17.73
26443	10.5	21.09	9.0	20.61	9.0	18.78	10.5	17.43
26595	11.3	21.80	5.9	18.04	7.4	17.67	11.2	17.74
26730	12.7	22.21	4.0	18.58	5.0	18.04	11.5	16.71
26793	11.7	21.79	5.7	18.41	6.8	17.68	12.0	16.50
26950	9.9	21.20	7.5	19.08	9.0	18.20	9.8	16.80
27049	10.0	21.66	5.3	17.31	7.2	17.62	9.4	17.27
27063	11.2	21.90	6.9	18.19	7.0	17.97	10.8	17.61
27121	12.7	22.05	5.3	18.35	6.6	17.86	11.8	16.91
27351	12.7	21.70	5.3	18.14	6.3	17.45	11.6	16.66
27483	11.3	21.65	6.4	18.93	8.0	18.37	10.6	16.34
27497	10.3	21.56	5.9	19.10	7.4	18.39	10.7	16.22
27659	12.1	21.74	7.9	19.58	8.7	17.94	12.0	16.72
27914	12.0	21.85	7.8	19.50	8.5	18.64	11.7	17.15
27916	12.5	22.02	6.2	18.26	9.5	18.11	10.8	16.41

27981	12.0	21.89	4.0	17.56	7.8	17.36	12.6	16.48
28010	12.8	21.55	6.8	18.68	8.0	17.60	12.4	16.70
28094	11.8	21.25	6.8	18.79	9.9	17.86	11.7	16.49
28105	10.5	21.39	5.7	18.40	8.0	16.82	10.9	16.74
28161	12.4	22.15	4.8	17.66	4.8	17.48	10.9	15.67
28187	12.0	22.08	3.8	17.35	5.8	17.17	12.2	16.47
28221	11.7	21.85	5.3	18.12	6.7	17.53	11.3	16.42
28247	12.8	22.02	6.9	18.75	8.9	17.63	12.0	17.81
28287	9.4	21.54	5.1	18.07	6.8	18.19	10.1	17.07
28415	11.4	21.89	4.5	17.58	6.8	18.00	9.9	16.19
28703	11.0	21.71	5.7	17.91	7.8	17.69	11.3	16.87
29264	11.1	21.89	4.6	17.72	7.9	17.32	10.7	16.51
29291	11.0	21.93	5.3	16.90	7.2	16.44	11.3	16.39
29394	11.4	21.70	5.7	19.18	8.1	18.87	10.1	16.59
29417	12.0	21.66	6.0	19.29	9.0	18.02	12.9	16.66
29432	11.6	21.99	4.7	18.03	4.7	18.01	11.3	15.93
29447	12.6	22.18	5.7	17.99	7.0	17.79	12.5	17.18
29537	10.9	21.49	5.9	18.42	9.0	17.14	10.0	17.37
29691	10.0	21.78	2.9	16.21	4.6	17.48	9.4	15.55
29731	11.7	21.65	5.7	17.70	6.9	17.70	11.9	16.46
29938	10.6	21.86	4.6	17.06	7.9	16.99	10.8	16.94
29986	10.1	21.81	5.7	18.16	7.4	17.62	9.3	16.73
30236	9.3	21.60	6.2	18.13	8.5	17.96	9.6	16.67
30367	10.2	21.59	5.0	17.11	7.0	17.54	10.3	17.53
30449	12.0	22.11	6.1	18.31	8.7	17.75	11.0	16.61
30577	12.0	21.80	7.7	19.44	8.0	18.47	11.2	17.58
30680	12.2	21.66	6.8	18.46	8.2	17.59	12.0	16.73
30778	10.6	21.64	6.1	18.21	8.4	17.93	10.6	16.58
30988	9.9	21.71	5.8	18.10	8.0	18.40	9.4	17.06
31043	11.8	21.82	7.0	18.51	8.8	18.04	11.7	17.29
31105	10.0	21.81	3.9	16.41	8.3	17.71	10.0	17.13
31194	10.0	21.80	4.1	16.80	8.7	18.09	9.7	17.46
31530	10.7	21.71	7.0	18.31	8.0	18.35	10.8	17.26
31678	10.0	21.45	5.6	17.47	7.3	17.26	10.9	17.46
31786	12.9	21.99	5.7	18.27	8.7	17.49	11.4	16.96
32090	11.0	21.24	8.7	19.85	9.9	18.44	12.0	17.33
32106	13.6	21.41	7.0	18.67	7.9	17.61	13.5	17.48
32192	10.9	21.98	5.5	17.12	6.8	17.86	9.7	17.51
32244	10.7	21.84	7.8	19.23	9.0	18.45	10.0	17.23
32569	10.0	21.60	5.9	18.35	9.9	18.35	10.6	17.35
33022	10.4	21.77	6.2	18.06	7.0	18.04	9.9	16.21
33161	8.7	21.64	3.7	15.24	6.9	18.05	8.6	17.29
33167	10.0	21.66	5.3	17.54	7.3	17.57	10.7	17.52

33276	9.4	21.35	6.3	17.77	8.9	17.69	10.4	17.53
33310	10.0	21.54	6.4	17.95	9.6	18.14	10.0	17.10
33445	11.0	22.07	2.9	15.81	5.8	17.16	9.7	16.80
33595	12.0	21.53	9.2	18.63	10.0	18.19	11.9	17.16
33677	11.6	21.93	4.9	17.94	6.6	17.69	10.0	16.49
33687	10.8	21.74	6.8	18.35	8.6	18.03	10.4	17.51
33750	10.2	21.35	6.5	18.65	8.6	18.06	11.6	17.59
34199	12.0	21.56	7.9	19.41	8.8	18.44	11.8	17.03
34358	10.5	21.83	5.1	18.24	7.3	17.93	8.8	16.57
34444	10.9	21.33	7.8	18.80	9.0	18.38	10.6	16.46
34491	11.1	21.22	6.7	19.25	8.5	17.86	11.7	16.49
34578	11.5	22.07	4.8	18.44	6.0	18.52	10.6	15.53
34903	11.8	21.81	7.6	19.06	8.8	18.21	11.2	17.02
34968	10.0	21.76	5.8	17.27	6.6	17.51	9.8	17.39
35148	11.2	21.55	8.4	19.88	9.4	18.43	9.0	16.57
35194	11.9	21.52	7.0	19.13	10.5	18.89	12.8	17.82
35276	11.8	21.87	6.1	18.28	8.3	18.01	10.7	16.59
35550	12.6	21.97	5.7	17.43	7.4	17.78	11.0	16.75
35724	11.4	22.02	5.7	17.65	6.0	17.87	9.7	16.57
35773	11.8	21.85	7.4	17.81	8.2	17.40	11.4	17.70
35851	13.1	21.57	5.9	18.43	7.5	17.40	12.0	16.67
35870	11.5	21.61	6.9	18.98	8.5	16.98	11.5	17.07
35941	12.2	21.94	6.6	18.53	8.8	17.73	11.2	17.22
36084	10.7	21.77	6.6	19.01	7.1	18.54	10.2	16.57
36207	12.9	21.78	8.3	19.53	10.4	18.43	11.6	17.35
36216	12.6	21.66	7.0	19.36	9.8	18.14	11.9	16.96
36265	11.8	21.91	6.7	19.11	8.8	18.63	11.1	17.30
36379	11.9	22.08	6.8	18.69	7.9	18.29	10.9	17.02
36426	12.0	21.87	6.5	18.77	9.9	18.32	11.3	17.49
36569	11.3	22.05	5.6	17.95	7.0	17.73	10.3	16.72
36699	10.7	21.99	5.4	17.22	7.0	17.19	9.6	16.39
36705	9.0	21.71	4.5	16.14	5.6	16.94	9.3	17.01
36727	10.5	21.95	6.6	17.71	7.4	17.39	9.1	17.28
36797	10.6	21.92	6.8	18.20	7.9	18.57	9.5	16.96
37052	10.8	21.99	2.9	16.68	5.7	17.53	10.2	16.11
37054	10.9	22.11	4.1	16.60	6.0	17.60	9.5	16.53
37264	10.9	21.73	7.8	19.21	8.0	18.57	10.1	16.67
37328	11.8	21.88	5.5	17.12	7.2	17.73	11.3	16.31
37416	11.2	21.98	4.5	17.86	6.9	17.77	9.6	16.18
37452	11.4	22.03	5.9	18.71	8.8	17.99	11.0	17.82
37595	12.0	22.05	5.0	17.96	7.8	17.29	11.9	16.90
37626	11.7	21.79	6.4	19.40	9.1	18.27	11.7	16.56
37702	11.8	21.99	6.2	19.81	7.0	19.08	11.7	16.22

37904	12.1	22.07	5.1	18.35	6.7	18.06	11.9	16.75
37919	11.9	21.55	9.0	20.26	9.8	18.78	11.0	17.40
37981	10.0	21.74	5.9	18.45	7.0	18.06	9.9	17.56
37999	12.3	21.92	5.6	18.63	7.8	17.20	11.5	17.09
38220	10.1	21.86	3.5	15.79	6.5	17.28	9.7	16.30
38353	12.0	22.24	4.3	17.63	6.9	17.27	11.1	17.34
38410	12.0	22.15	5.0	17.42	6.0	18.12	11.3	16.38
38526	11.8	22.08	5.5	18.40	6.0	18.35	10.9	16.43
38542	12.0	21.82	6.9	19.29	8.9	18.53	11.2	17.29
38686	10.0	21.96	3.1	15.68	6.8	16.47	9.5	17.28
38719	12.7	22.08	4.8	18.16	6.7	17.97	11.5	16.08
38912	12.0	21.75	6.9	18.89	6.4	17.95	10.9	16.75
38966	10.0	21.72	4.6	16.67	7.5	17.27	9.2	17.35
38988	11.5	22.01	5.5	16.71	7.1	17.46	11.7	17.65
39039	10.4	21.67	4.7	16.89	9.1	17.37	10.0	17.02
39062	11.8	21.71	5.6	17.27	8.9	17.77	11.3	17.21
39063	11.5	21.89	5.1	17.71	7.3	17.89	10.4	17.00
39331	10.4	21.63	5.2	17.23	8.5	17.49	10.0	17.43
39378	11.0	21.91	3.5	15.76	6.3	16.75	10.4	17.55
39461	11.7	22.09	3.4	16.20	6.7	17.35	11.6	16.98
39464	9.7	21.79	3.7	16.86	5.5	17.65	10.1	17.09
39506	11.7	21.88	5.7	17.54	8.6	16.79	10.4	16.26
39647	13.0	21.99	6.9	18.59	8.7	18.41	12.4	17.50
39692	11.5	22.03	6.4	17.96	7.0	18.08	11.2	17.15
39721	10.7	21.69	5.9	18.40	6.0	17.82	11.3	16.60
39965	12.9	21.74	6.8	18.62	9.3	17.27	11.9	17.09
39979	11.7	22.02	5.9	18.50	8.9	17.68	10.9	17.21
40076	11.6	21.79	6.0	18.23	7.7	17.19	10.1	16.91
40224	11.9	22.03	5.4	17.63	7.8	17.26	11.7	16.62
40383	10.0	21.78	3.7	16.49	6.0	17.45	7.8	16.29
40419	12.4	22.28	4.6	18.53	5.1	17.82	12.4	16.40
40921	13.0	21.63	6.0	18.68	8.3	17.76	12.7	17.63
40946	13.1	22.23	3.7	17.83	6.7	17.53	12.2	16.58
41071	12.6	21.96	5.2	17.13	6.9	17.76	12.9	17.15
41092	11.3	22.09	5.3	17.79	5.6	17.81	11.3	16.36
41101	11.1	22.09	3.3	16.65	5.0	17.49	9.9	16.06
41142	13.0	22.29	3.5	16.91	5.0	16.67	11.6	16.16
41287	12.3	22.09	4.5	17.59	5.9	17.26	11.3	16.40
41392	12.7	22.20	4.8	18.15	5.0	17.84	10.9	16.34
41432	10.9	21.95	5.8	17.45	6.8	17.67	10.3	16.19
41488	9.9	21.82	4.2	17.82	7.7	17.86	10.5	17.01
41691	12.9	22.24	4.4	17.64	6.4	17.91	12.6	16.63
41735	12.0	22.11	5.2	18.01	8.8	17.90	12.0	16.67

42017	13.5	22.33	4.0	17.67	4.1	17.61	12.1	15.70
42137	11.5	22.17	4.7	17.53	6.7	17.23	11.1	16.11
42458	11.5	21.60	5.7	18.31	8.7	17.92	11.9	16.31
42626	11.1	21.73	7.8	19.30	8.0	18.55	10.9	17.32
42956	11.2	21.66	7.8	19.86	9.7	18.73	11.0	16.74
43213	13.9	21.75	6.5	18.23	7.0	17.47	13.3	16.90
43274	13.3	22.24	4.9	18.55	6.6	17.75	12.7	16.45
43297	11.7	21.80	4.7	18.17	8.5	17.67	11.5	17.34
43331	12.5	21.92	6.8	19.25	7.4	18.21	11.9	17.53
43465	12.5	21.93	6.7	19.07	7.0	18.24	11.5	16.36
43480	12.1	21.39	7.8	19.75	8.8	18.15	12.3	17.16
43547	12.4	20.77	6.9	19.36	8.7	17.28	13.1	16.40
43635	11.0	21.83	5.7	18.09	7.0	18.02	10.9	16.71
43871	12.3	22.30	4.9	17.36	6.3	17.09	10.6	16.36
43905	13.8	21.88	7.0	18.81	7.6	17.42	12.5	17.72
43938	12.4	22.11	3.5	17.25	6.9	16.88	13.0	16.65
43998	12.9	21.91	6.9	19.10	7.9	17.86	11.2	16.44
44304	10.3	21.94	6.4	18.00	7.0	18.20	10.6	17.59
44673	12.3	21.61	5.9	18.72	8.3	17.82	12.8	17.28
44703	11.8	21.69	5.8	18.76	7.2	17.46	11.1	16.34
44878	13.4	21.73	5.6	17.89	7.6	17.10	13.1	17.27
45146	12.1	21.84	7.0	19.57	7.9	18.18	12.3	16.85
45168	11.9	21.51	7.6	19.77	8.6	18.23	12.0	17.10
45300	11.3	21.88	6.8	18.40	7.6	18.19	11.8	16.62
45527	12.8	21.79	7.8	18.83	8.0	18.00	12.3	17.30
46101	11.9	21.70	6.9	19.16	8.0	18.00	9.6	17.18
46574	12.8	21.18	7.0	19.45	8.4	17.98	12.5	17.19
46640	12.0	21.48	7.8	19.46	8.0	18.19	12.3	17.35
46754	8.9	18.30	7.8	18.59	8.0	17.62	9.4	16.36
46791	12.9	21.76	5.9	18.04	7.6	16.94	11.7	16.15
46962	13.1	21.60	6.1	19.61	6.9	17.97	12.6	16.94
47005	13.4	21.94	5.9	18.47	6.9	17.55	11.3	16.27
47015	11.7	21.73	6.9	19.32	9.2	18.12	11.6	16.47
47040	12.0	21.84	6.9	19.07	9.3	18.07	11.7	16.44
47201	11.9	21.77	7.3	19.25	7.9	17.98	11.5	16.75
47234	12.9	21.86	6.5	19.44	7.0	18.63	12.3	16.51
47333	10.9	21.98	4.5	17.15	6.9	17.37	11.3	16.64
47409	12.1	22.18	4.9	18.17	7.5	18.12	12.0	16.45
47513	12.0	21.89	6.7	19.31	8.7	18.35	12.0	16.45
47527	12.9	21.79	7.8	19.69	9.9	18.31	13.0	16.85
47694	11.0	21.65	6.5	17.99	7.9	17.49	10.0	16.33
47695	10.9	21.86	4.5	17.53	8.3	18.11	10.7	16.96
47868	11.6	21.92	4.0	16.17	5.5	16.45	10.2	16.41

47883	12.0	21.47	7.0	19.97	10.2	17.85	10.5	16.54
48180	11.0	21.39	7.8	20.08	8.2	18.60	9.2	16.66
48312	11.7	21.76	5.8	18.66	6.6	17.66	10.5	15.97
48571	11.6	21.89	5.2	18.35	7.0	18.46	11.4	16.86
48611	12.0	21.87	7.6	19.54	8.8	18.96	11.9	16.86
48719	12.0	21.58	8.0	19.44	9.9	18.31	8.7	17.73
48846	10.3	21.62	6.1	18.47	7.0	18.22	10.4	17.38
49101	11.5	21.85	5.5	18.39	7.9	18.27	10.8	16.99
49108	9.1	21.31	6.2	19.12	8.0	18.72	9.0	16.24
49157	12.8	22.18	2.2	16.81	5.0	16.21	11.6	15.94
49211	10.8	22.10	2.4	15.44	6.4	16.49	9.1	17.22
49296	10.1	21.89	3.9	17.43	6.0	17.61	9.9	16.46
49334	11.5	22.02	3.7	16.85	5.1	16.78	12.0	15.99
49411	12.1	22.14	3.9	16.86	5.7	17.42	11.1	15.93
49488	12.6	22.36	2.6	16.14	4.7	16.50	10.1	15.09
49649	13.4	22.51	2.8	15.92	3.9	16.70	12.3	15.31
49774	12.8	22.31	4.0	17.78	5.3	17.40	11.1	15.30
49907	12.7	22.31	3.2	16.63	5.6	17.38	10.2	16.64
49918	10.7	21.80	4.1	16.63	6.9	16.73	9.3	16.70
49963	9.8	21.94	1.6	15.96	4.9	16.05	10.0	16.70
49971	11.1	21.94	3.4	16.83	4.9	17.30	10.2	15.96
50082	9.9	21.81	2.9	15.59	6.5	17.16	11.0	16.31
50129	10.4	21.98	4.7	17.99	6.4	17.84	10.4	21.98
50249	11.0	21.76	5.9	18.28	8.0	18.01	9.6	16.74
50306	10.9	22.01	6.0	17.58	7.2	17.70	8.9	17.54
50319	8.8	21.70	3.4	16.54	7.8	18.16	8.0	16.96
50406	8.0	21.36	3.6	15.82	7.8	18.15	7.9	17.22
50431	10.8	22.04	2.7	16.42	4.9	17.24	9.0	15.76
50515	8.4	21.45	2.8	15.81	4.9	16.90	11.7	17.27
50529	8.8	21.56	4.3	16.63	7.0	17.67	7.8	16.45
50562	7.6	21.08	1.8	12.90	5.6	16.93	7.9	16.97
50794	9.7	21.81	0.8	13.94	5.6	16.89	9.5	16.17
50809	9.5	22.02	1.8	14.42	4.2	16.25	9.2	16.20
50848	9.0	21.69	2.3	14.41	6.6	17.17	8.7	16.50
50933	10.7	22.01	0.3	15.04	4.8	16.43	9.8	15.87

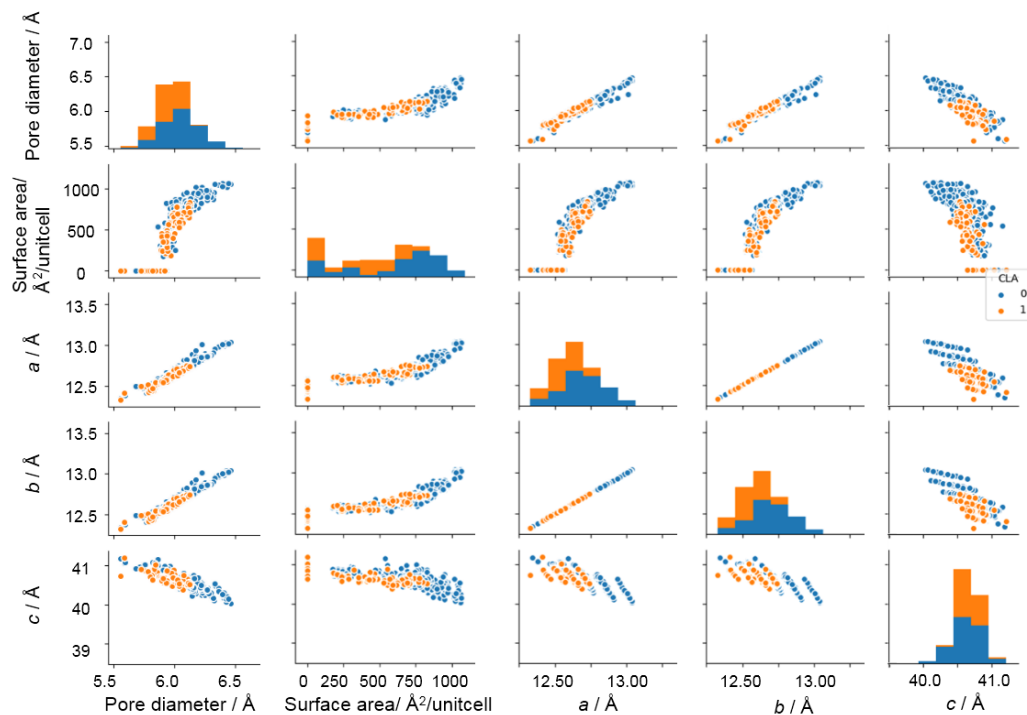


Figure S1. The scatter matrices of five features (structure parameters of zeolites, a , b and c , the pore diameters p , and accessible surface area s) for the adsorption of DMSO₂.

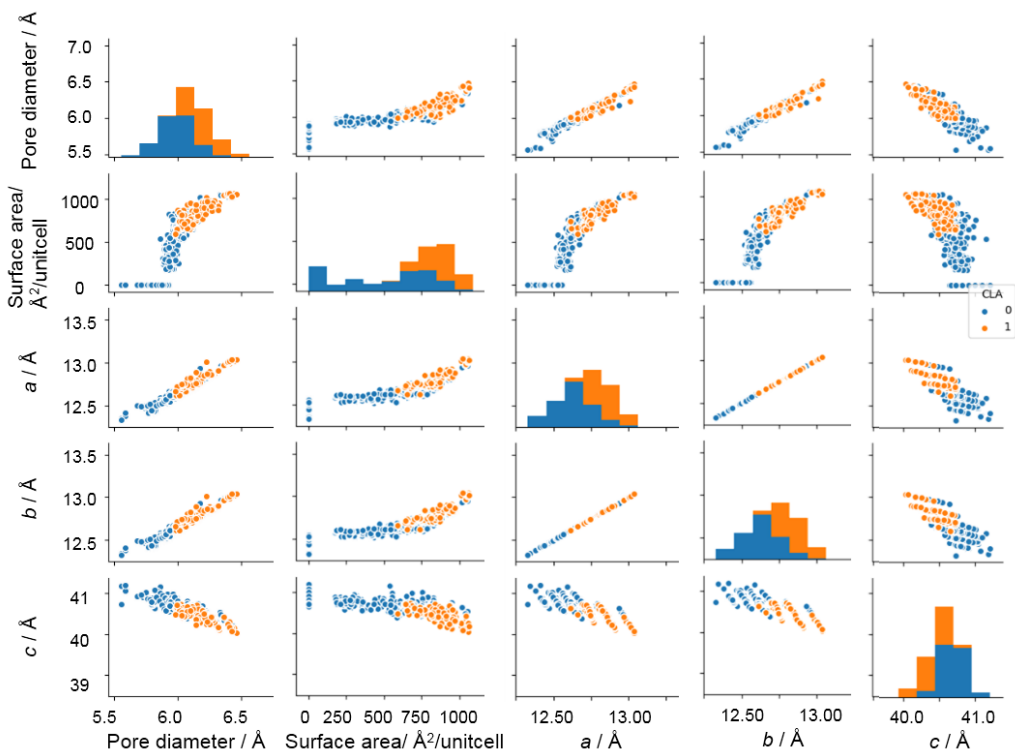


Figure S2. The scatter matrices of five features (structure parameters of zeolites, a , b and c , the pore diameters p , and accessible surface area s) for the adsorption of TMS.

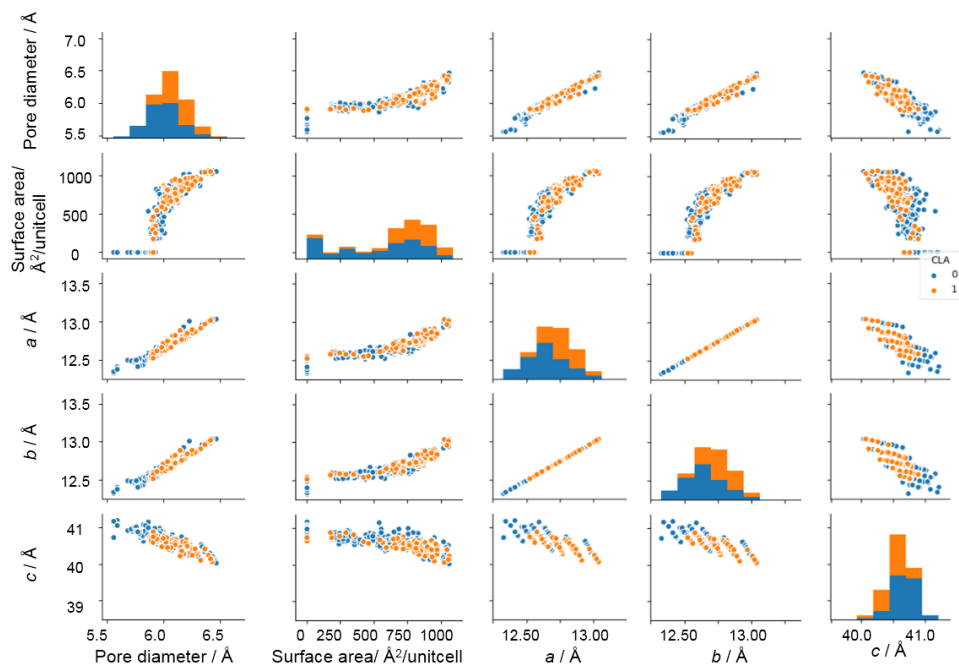


Figure S3. The scatter matrices of five features (structure parameters of zeolites, a , b and c , the pore diameters p , and accessible surface area s) for the adsorption of DMSD.

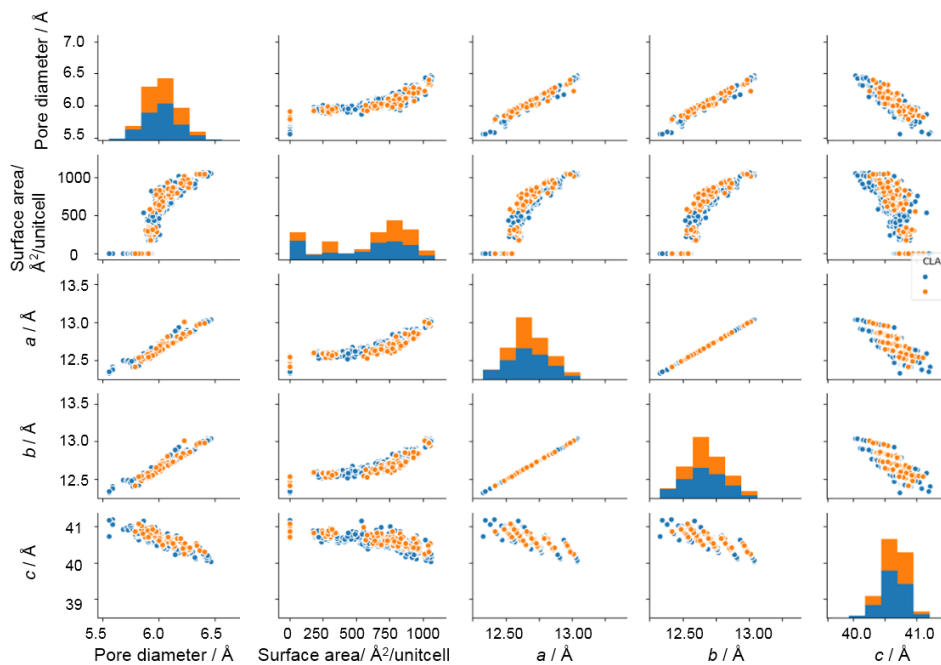


Figure S4. The scatter matrices of five features (structure parameters of zeolites, a , b and c , the pore diameters p , and accessible surface area s) for the adsorption of MMST.

Table S2. The identification numbers, adsorption energy, pore diameters (p), accessible surface area (s), crystal parameters (a , b , and c) of the top 10 pure silica zeolites for the adsorption of DMSO₂ screened by GCMC simulations.

Num.	Adsorption Energy (kcal/mol)	Pore Diameter (Å)	Surface Area (Å ² /unitcell)	a (Å)	b (Å)	c (Å)
49649	22.51	5.82	0.00	12.47	12.47	40.64
49488	22.36	5.80	0.00	12.45	12.45	40.72
42017	22.33	6.04	528.23	12.66	12.66	40.55
49907	22.31	5.91	353.09	12.54	12.54	40.67
49774	22.31	5.93	353.74	12.57	12.57	40.56
43871	22.30	5.94	426.78	12.55	12.55	40.63
8463	22.29	5.94	288.29	12.58	12.58	40.64
41142	22.29	5.94	241.46	12.56	12.56	40.58
40419	22.28	5.90	415.53	12.55	12.55	40.62
38353	22.24	5.90	237.35	12.54	12.54	40.70

Table S3. The identification numbers, adsorption energy, pore diameters (p), accessible surface area (s), crystal parameters (a , b , and c) of the top 10 pure silica zeolites for the adsorption of TMS screened by GCMC simulations.

Num.	Adsorption Energy (kcal/mol)	Pore Diameter (Å)	Surface Area (Å ² /unitcell)	a (Å)	b (Å)	c (Å)
26443	20.61	6.14	930.33	12.89	12.89	40.24
24553	20.36	6.23	968.97	12.87	12.87	40.31
13981	20.35	6.42	1021.39	13.04	13.04	40.07
11718	20.34	6.41	1061.37	13.02	13.02	40.16
37919	20.26	6.27	913.76	12.86	12.86	40.43
26405	20.18	6.03	810.00	12.74	12.74	40.47
13887	20.10	6.10	954.03	12.82	12.82	40.57
48180	20.08	6.05	714.50	12.75	12.75	40.44
6831	20.07	6.40	1059.75	13.00	13.00	40.25
6333	20.03	6.42	1051.39	13.02	13.02	40.16

Table S4. The identification numbers, adsorption energy, pore diameters (p), accessible surface area (s), crystal parameters (a , b , and c) of the top 10 pure silica zeolites for the adsorption of DMSD screened by GCMC simulations.

Num.	Adsorption Energy (kcal/mol)	Pore Diameter (Å)	Surface Area (Å ² /unitcell)	a (Å)	b (Å)	c (Å)
37702	19.08	5.99	591.82	12.66	12.66	40.49
12791	19.05	6.25	877.66	12.89	12.89	40.26
26405	19.05	6.03	810.00	12.74	12.74	40.47
4138	18.97	6.28	926.70	12.87	12.87	40.42
48611	18.96	5.99	642.74	12.72	12.72	40.71
13771	18.94	6.21	897.28	12.85	12.85	40.51
35194	18.89	6.26	969.63	12.85	12.85	40.42
29394	18.87	6.06	664.39	12.66	12.66	40.47
13640	18.82	6.05	819.21	12.75	12.75	40.41
26443	18.78	6.14	930.33	12.89	12.89	40.24

Table S5. The identification numbers, adsorption energy, pore diameters (p), accessible surface area (s), crystal parameters (a , b , and c) of the top 10 pure silica zeolites for the adsorption of MMST screened by GCMC simulations.

Num.	Adsorption Energy (kcal/mol)	Pore Diameter (Å)	Surface Area (Å ² /unitcell)	a (Å)	b (Å)	c (Å)
50129	21.98	5.91	0.00	12.54	12.54	40.72
16501	18.40	5.95	319.07	12.56	12.56	40.92
18969	18.40	5.79	0.00	12.42	12.42	40.86
22323	18.28	5.92	579.44	12.53	12.53	40.78
17229	18.24	5.98	771.67	12.66	12.66	40.88
15359	18.19	6.00	637.63	12.63	12.63	40.62
4138	18.11	6.28	926.70	12.87	12.87	40.42
2469	18.10	6.13	869.02	12.73	12.73	40.54
17360	18.10	6.01	832.25	12.69	12.69	40.68
25913	18.05	6.04	686.29	12.65	12.65	40.50

List S1. The list of Machine-Learning-assist selected 230 prominent pure-silica zeolites.

121, 166, 208, 497, 690, 848, 870, 989, 1618, 1969, 2063, 2457, 2639, 2747, 2775,
3226, 3955, 4511, 5330, 5347, 5355, 5417, 5506, 5548, 5550, 5655, 5672, 5687, 5766,
5802, 5870, 5876, 6028, 6056, 6090, 6096, 6164, 6202, 6241, 6502, 6725, 6931, 6943,
6976, 6987, 8861, 8866, 8935, 9304, 9437, 9533, 9629, 9679, 9681, 10001, 10552,
10810, 10817, 10958, 11080, 11107, 11138, 11382, 11458, 11462, 11465, 11466, 11482,
11486, 11501, 11517, 11524, 11854, 11856, 12053, 12054, 12105, 12400, 12445, 12459,
12484, 12571, 12586, 12684, 12727, 13089, 13094, 13120, 13197, 13260, 13405,
13438, 13508, 13560, 13573, 13682, 13833, 13838, 13909, 13927, 15152, 15706,
15726, 15728, 15734, 24237, 25262, 25367, 25383, 25451, 26068, 26199, 26208,
26321, 26406, 26423, 26432, 26436, 26454, 26622, 26653, 26698, 26860, 26864,
26865, 26870, 26901, 26920, 26922, 26995, 27038, 27053, 27054, 27092, 27097,
27340, 27400, 27411, 27434, 27543, 27625, 27828, 27914, 27916, 28059, 28079,
28110, 28246, 28645, 28893, 28922, 29350, 29355, 29363, 29448, 30083, 30087,
30131, 30136, 30143, 30145, 30186, 30486, 30672, 30817, 30883, 30928, 30930,
30956, 31913, 31942, 31944, 32039, 32085, 33762, 33793, 33838, 33951, 33963,
34185, 34406, 34583, 35018, 35212, 35289, 35294, 35692, 35992, 36179, 36474,
36521, 36593, 36594, 37346, 37582, 37658, 37829, 38496, 38500, 38535, 38539,
38543, 38578, 38732, 38735, 38766, 38809, 38811, 38824, 38829, 38896, 39959,
39987, 40042, 40050, 40061, 40110, 40944, 41215, 41695, 43441, 43573, 43723,
43728, 45386, 45390, 45391, 45869, 46107, 46517

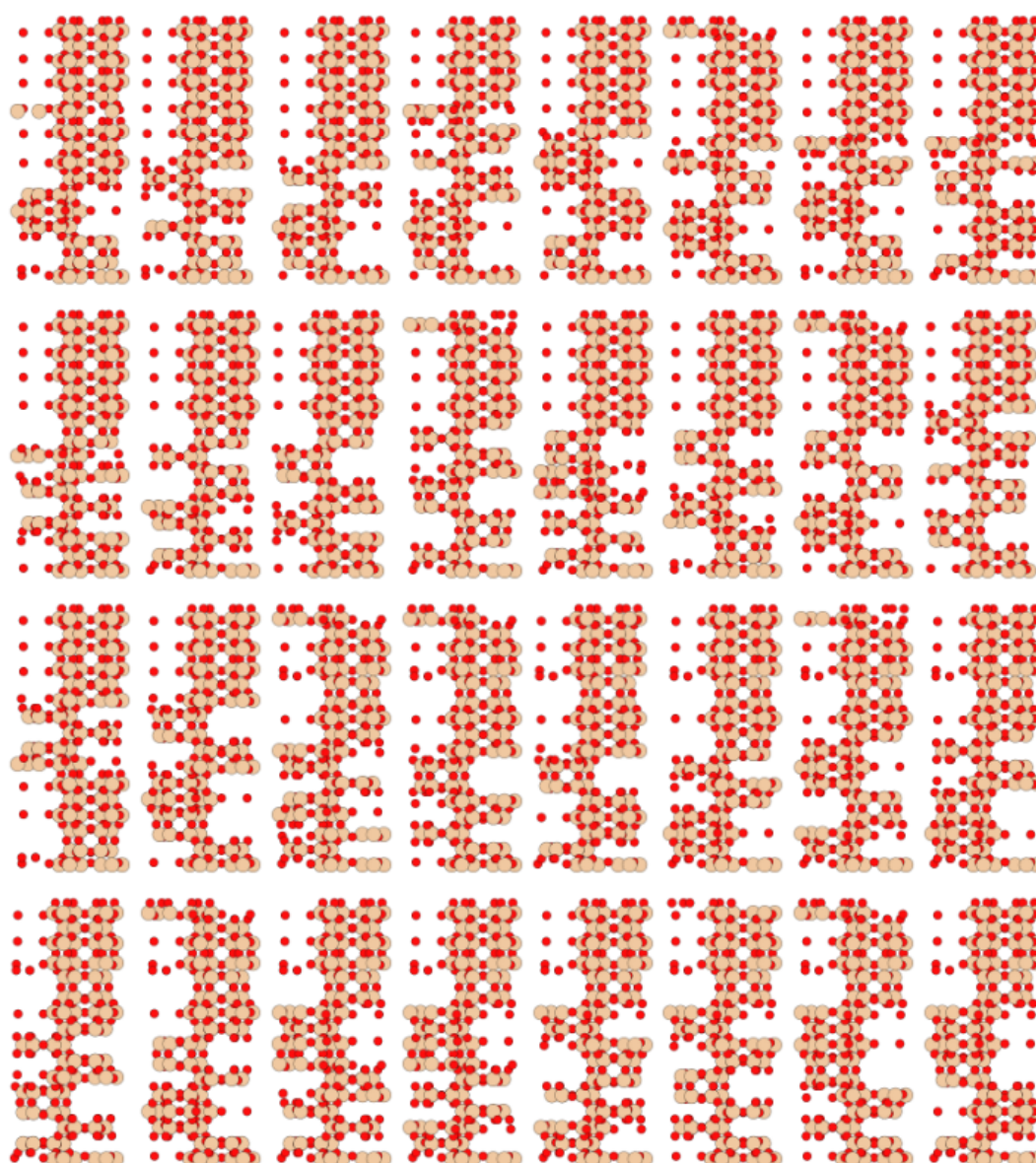


Figure S5. The structures of 230 (1st-32rd) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

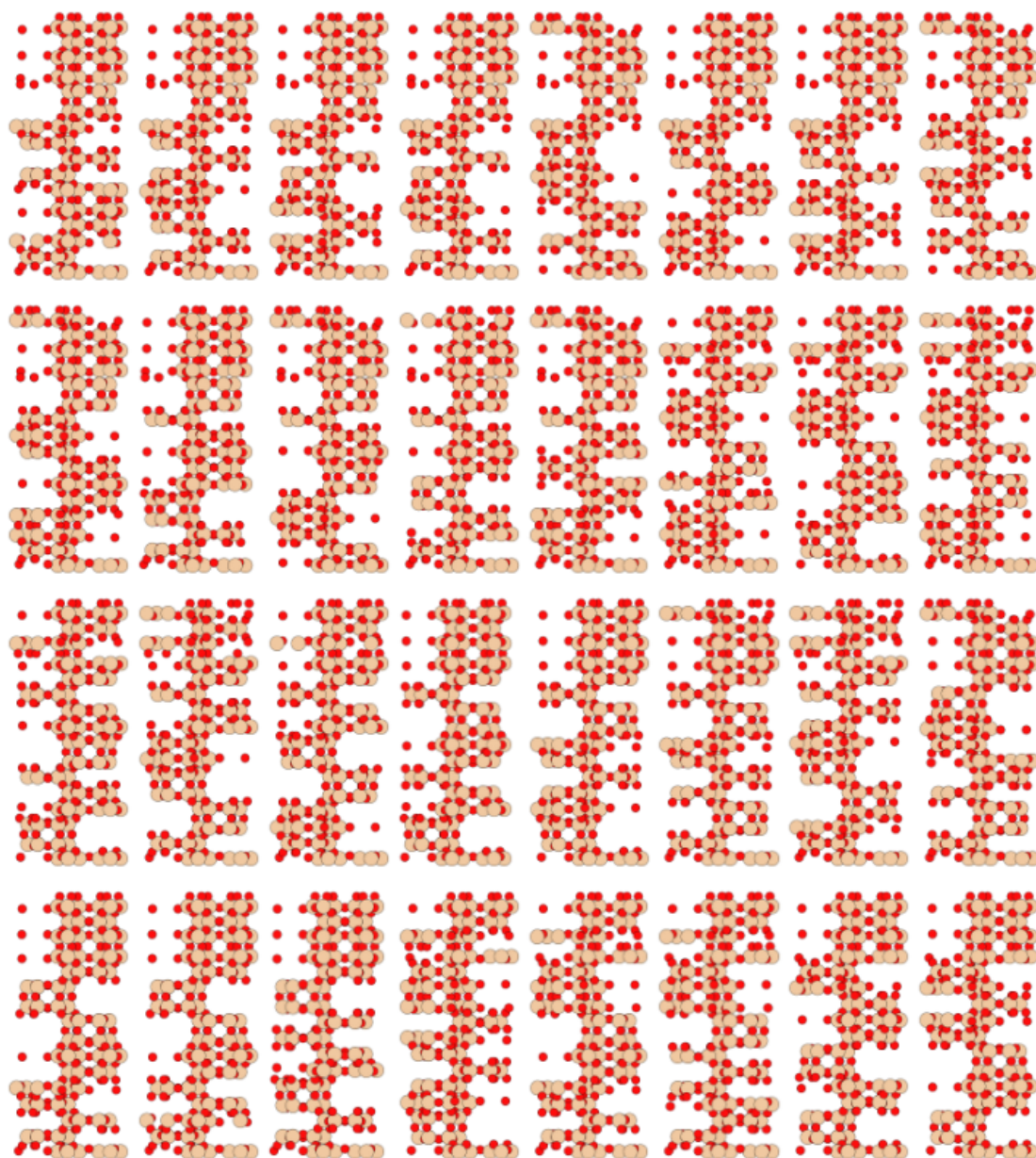


Figure S6. The structures of 230 (33th-64th) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

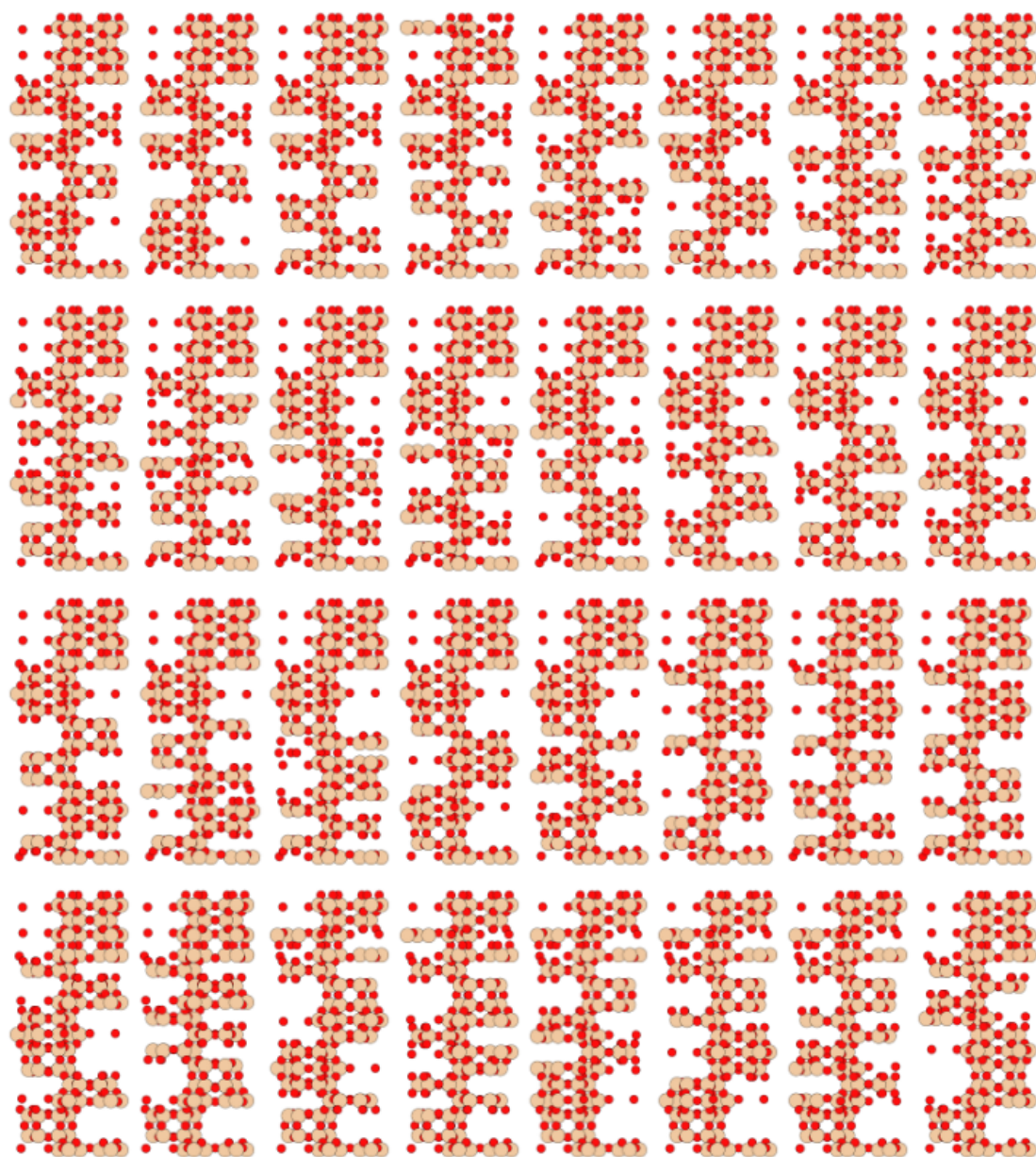


Figure S7. The structures of 230 (65th-96th) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

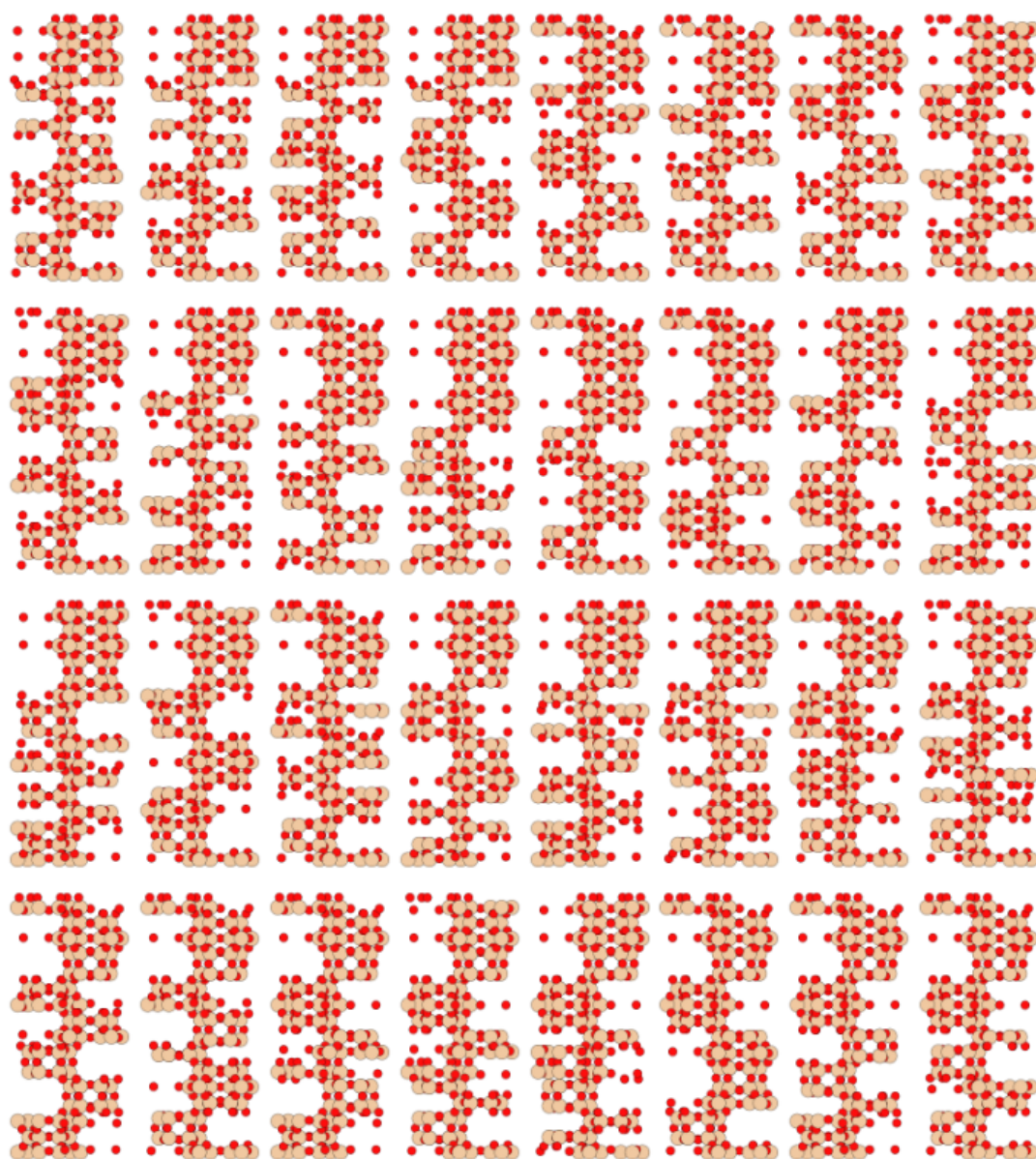


Figure S8. The structures of 230 (97th-128th) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

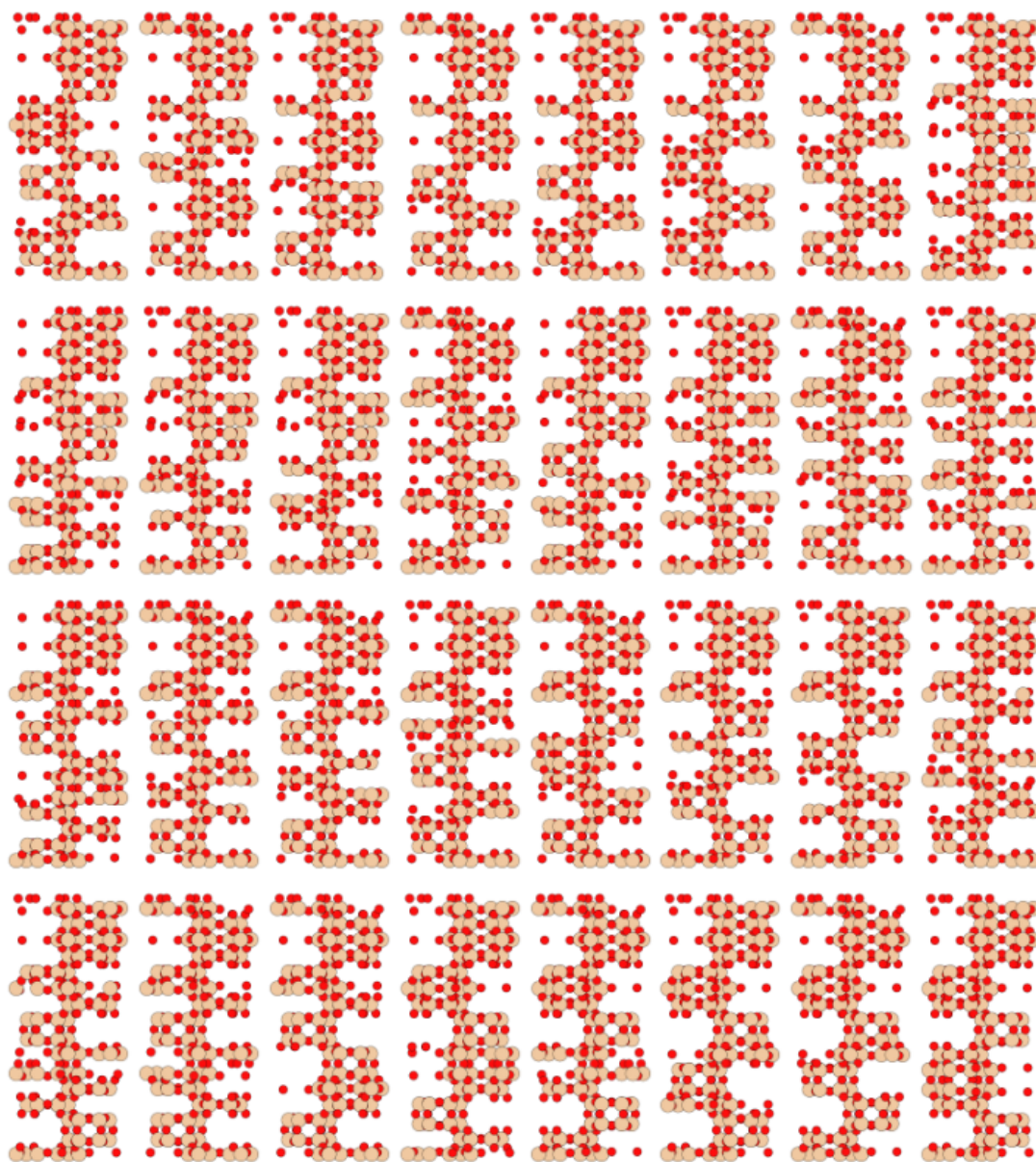


Figure S9. The structures of 230 (128th-160th) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

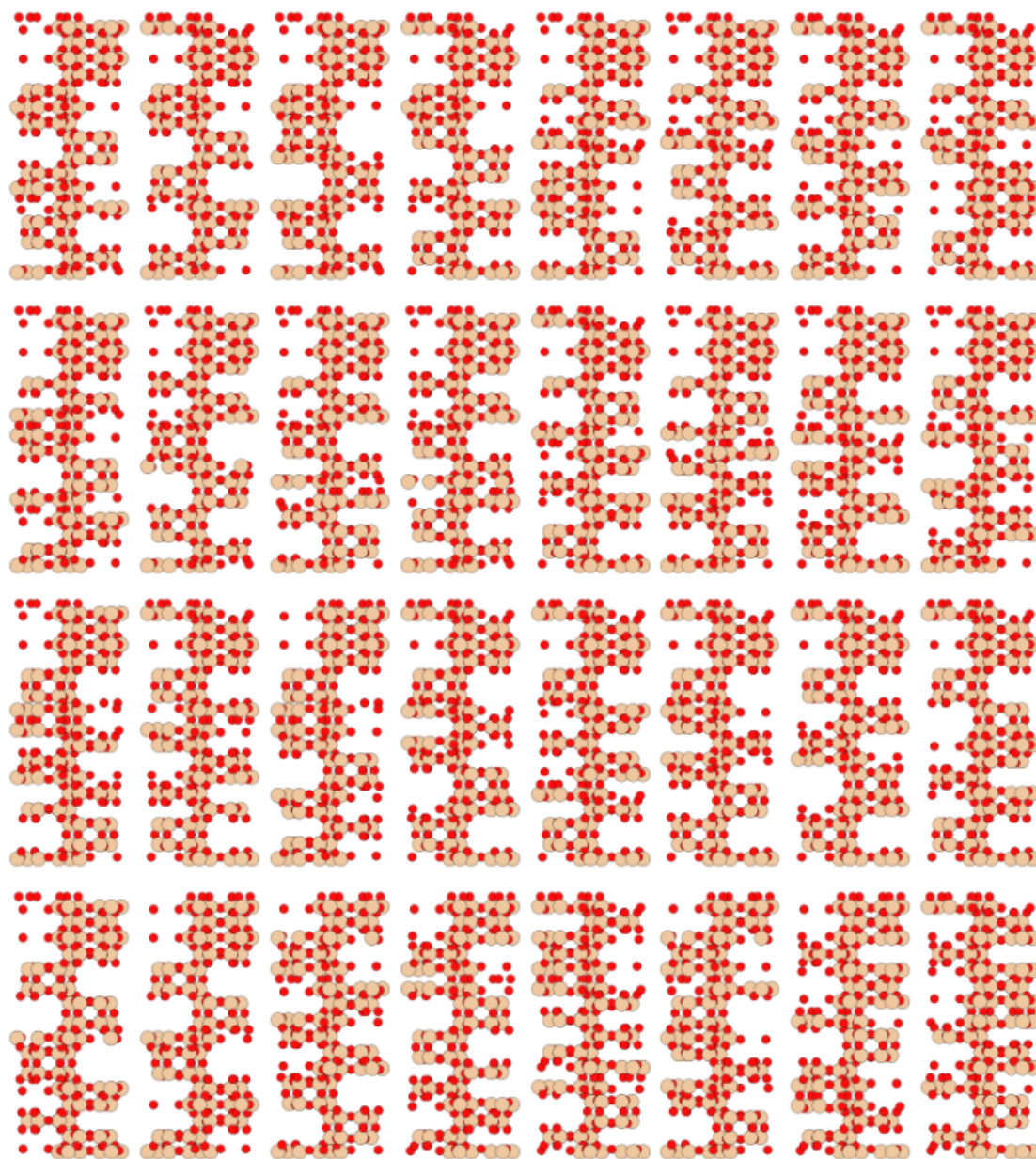


Figure S10. The structures of 230 (161th-192rd) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

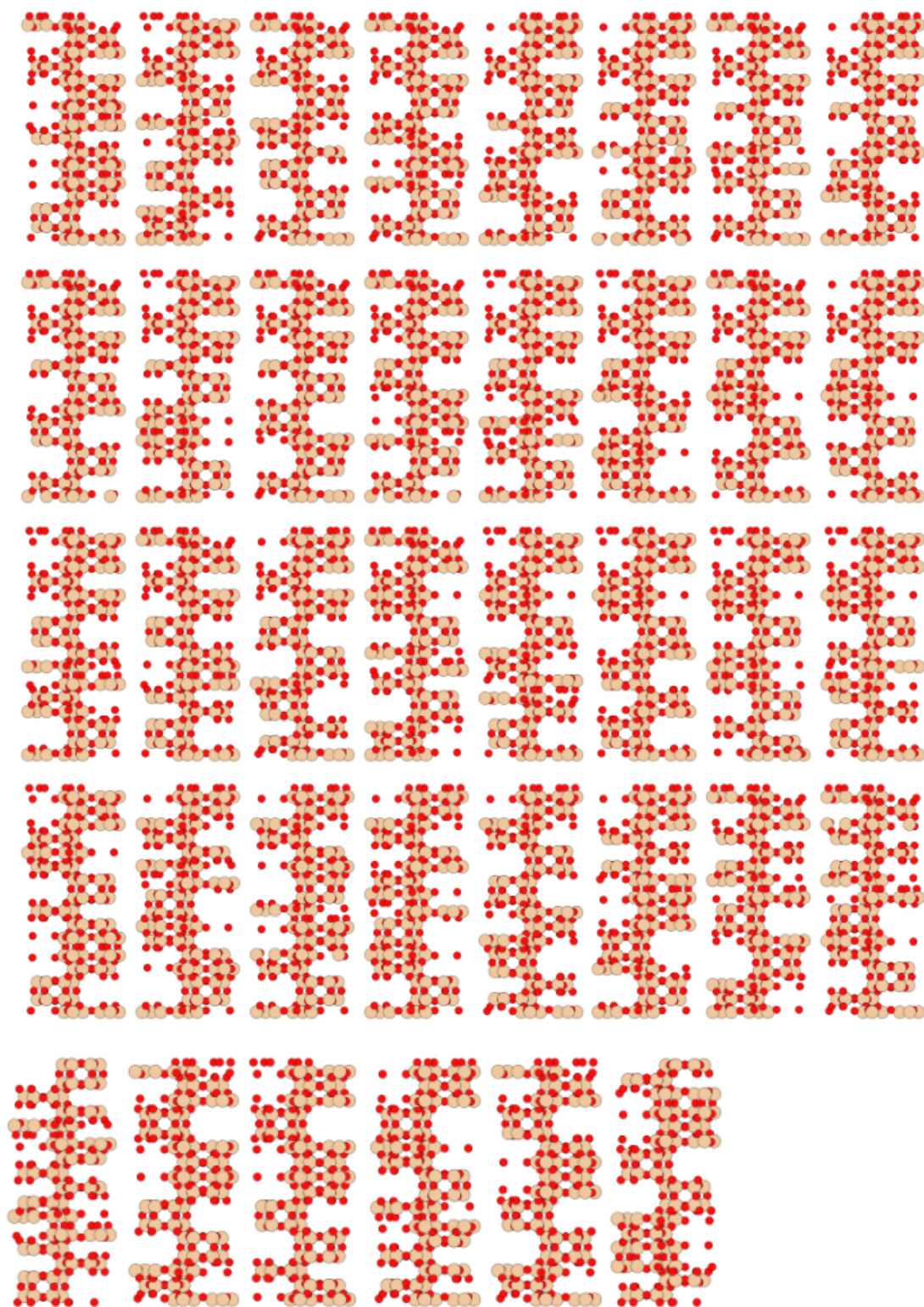


Figure S11. The structures of 230 (193th-230th) four-class-1 zeolites selected by ML algorithm. The order of these zeolites are following the order of List S1.

List S2. The list of two sets of 10 zeolites randomly selected to reconfirm the adsorption performance by GCMC simulations.

Set 1: 6164, 12105, 13909, 28509, 30131, 9629, 30143, 38239, 2457, 5355

Set 2: 30143, 6028, 5072, 28922, 26423, 5550, 30817, 8866, 989, 10001

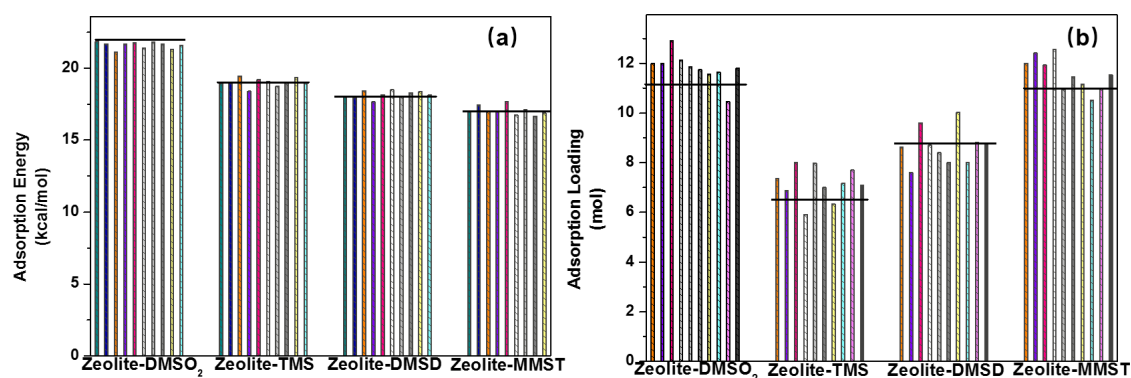


Figure S12. (a) The adsorption energies and (b) adsorption loading of the second set of randomly chosen 10 zeolites from the predicted 230 four-class-1 zeolites, where the upper lines correspond to the top 20% adsorption energies (a) and top 30% adsorption loading in the training data of 500.

The well-trained ML models and the randomly selected 500 structures have been uploaded in https://github.com/shirulin1026/ML_Screening_Zeolites. The model files can be downloaded and employed for predictions through scikit-learn package.