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Supplementary to "Theoretical Study on the Gas Adsorption Capacity and Selectivity of CPM-200-In/Mg and CPM-200-In/Mg-X (-X = -NH2, -OH, -N, -F)"

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Table S1. XYZ coordinate of the CPM-200-In/Mg-NH2(site2)(a=22.97 b=c=22.30β=α=γ=90)

Atom	Element	X	Y	Z
Mg1	Mg	0.16881	0.24019	0.70107
C_benz1	C	0.31848	0.2185	0.45874
C_benz4	C	0.28527	0.22093	0.51378
C_benz1	C	0.31654	0.21835	0.56933
C_benz2	C	0.37732	0.21604	0.56869
C_benz3	C	0.40985	0.21524	0.51557
C_benz2	C	0.37928	0.21555	0.46068
C_COO	C	0.28706	0.21789	0.62853
C_COO	C	0.28966	0.2203	0.3989
O_COO2	O	0.23519	0.23622	0.39809
O_COO1	O	0.31817	0.20714	0.35227
O_COO1	O	0.32197	0.21257	0.67355
O_COO2	O	0.23209	0.2227	0.63416
N1	N	0.47078	0.21448	0.52389
N_2	N	0.22685	0.22427	0.51407
H_benz	H	0.40052	0.21505	0.61128
H_benz	H	0.4034	0.21417	0.4186
Mg1	Mg	0.80544	0.76164	0.6901
C_benz1	C	0.65169	0.77034	0.45369
C_benz4	C	0.68647	0.77059	0.50771
C_benz1	C	0.65813	0.78264	0.56414
C_benz2	C	0.59738	0.78706	0.56533
C_benz3	C	0.56282	0.78298	0.51356
C_benz2	C	0.59137	0.77679	0.4578
C_COO	C	0.69077	0.78886	0.622
C_COO	C	0.67859	0.76448	0.39244
O_COO2	O	0.73106	0.74402	0.38772
O_COO1	O	0.64823	0.77982	0.34729
O_COO1	O	0.66187	0.80543	0.66811
O_COO2	O	0.74566	0.77696	0.62388
N1	N	0.50199	0.7849	0.52346
N_2	N	0.74432	0.76114	0.50533
H_benz	H	0.57551	0.79334	0.60823
H_benz	H	0.56548	0.77579	0.41685
Mg1	Mg	0.80302	0.24027	0.29892
C_benz1	C	0.65347	0.21862	0.54103
C_benz4	C	0.68654	0.22115	0.4859
C_benz1	C	0.65516	0.21845	0.43044
C_benz2	C	0.59439	0.21604	0.4312

C_benz3	C	0.56198	0.21527	0.48439
C_benz2	C	0.59266	0.21562	0.53922
C_COO	C	0.68463	0.21794	0.37126
C_COO	C	0.68236	0.22032	0.60084
O_COO2	O	0.73679	0.23641	0.60171
O_COO1	O	0.65391	0.20697	0.64745
O_COO1	O	0.64977	0.21252	0.32619
O_COO2	O	0.7396	0.22275	0.36572
N1	N	0.50103	0.21445	0.47618
N_2	N	0.74495	0.22463	0.48524
H_benz	H	0.57104	0.21497	0.3887
H_benz	H	0.56868	0.21416	0.58138
Mg1	Mg	0.16653	0.76169	0.31004
C_benz1	C	0.32021	0.77036	0.54644
C_benz4	C	0.28549	0.77067	0.49235
C_benz1	C	0.3139	0.78272	0.43597
C_benz2	C	0.37466	0.78713	0.43484
C_benz3	C	0.40915	0.78302	0.48665
C_benz2	C	0.38054	0.77682	0.54238
C_COO	C	0.28127	0.78893	0.37809
C_COO	C	0.29338	0.7644	0.60771
O_COO2	O	0.24093	0.74392	0.6125
O_COO1	O	0.32377	0.77971	0.65286
O_COO1	O	0.31018	0.80552	0.33198
O_COO2	O	0.22641	0.77697	0.37621
N1	N	0.46999	0.7849	0.47678
N_2	N	0.22763	0.76123	0.49449
H_benz	H	0.39656	0.79342	0.39196
H_benz	H	0.4064	0.77576	0.58334
In1	In	0.67384	0.1915	0.23558
C_benz1	C	0.42887	0.33069	0.21502
C_benz4	C	0.47729	0.28902	0.21419
C_benz1	C	0.53583	0.31272	0.21006
C_benz2	C	0.5436	0.37526	0.2076
C_benz3	C	0.49653	0.41566	0.2078
C_benz2	C	0.43965	0.3918	0.21097
C_COO	C	0.58768	0.27254	0.21212
C_COO	C	0.36687	0.31013	0.22343
O_COO2	O	0.35821	0.25636	0.24191
O_COO1	O	0.32522	0.34697	0.21346
O_COO1	O	0.63982	0.2923	0.20908
O_COO2	O	0.57989	0.21473	0.21889
N1	N	0.50917	0.47802	0.20776
N_2	N	0.46706	0.22967	0.21628

H_benz	H	0.58781	0.39316	0.20698
H_benz	H	0.40307	0.42278	0.21188
Mg1	Mg	0.68598	0.82132	0.75185
C_benz1	C	0.44508	0.66755	0.77878
C_benz4	C	0.499	0.7015	0.77681
C_benz1	C	0.55347	0.66978	0.78436
C_benz2	C	0.55197	0.60726	0.78979
C_benz3	C	0.50014	0.57364	0.78921
C_benz2	C	0.44714	0.60511	0.78481
C_COO	C	0.61192	0.70027	0.78532
C_COO	C	0.38606	0.69676	0.77397
O_COO2	O	0.38116	0.75254	0.76201
O_COO1	O	0.3417	0.66211	0.78218
O_COO1	O	0.656	0.66535	0.79701
O_COO2	O	0.61754	0.75607	0.77508
N1	N	0.50808	0.511	0.79219
N_2	N	0.49845	0.76122	0.76863
H_benz	H	0.59294	0.58288	0.7936
H_benz	H	0.40636	0.58014	0.78522
Mg1	Mg	0.28603	0.82143	0.24828
C_benz1	C	0.52697	0.66778	0.22115
C_benz4	C	0.47305	0.70172	0.22318
C_benz1	C	0.41856	0.67006	0.2155
C_benz2	C	0.42006	0.60755	0.20988
C_benz3	C	0.47188	0.57393	0.21035
C_benz2	C	0.52489	0.60537	0.21491
C_COO	C	0.36011	0.7005	0.21462
C_COO	C	0.58593	0.69699	0.22617
O_COO2	O	0.59084	0.75279	0.23805
O_COO1	O	0.63028	0.66227	0.21822
O_COO1	O	0.31603	0.66559	0.20284
O_COO2	O	0.35446	0.75627	0.225
N1	N	0.46397	0.51128	0.20726
N_2	N	0.47378	0.76142	0.23159
H_benz	H	0.37911	0.58316	0.206
H_benz	H	0.56566	0.58038	0.21442
In1	In	0.29822	0.19144	0.76421
C_benz1	C	0.5433	0.33043	0.78448
C_benz4	C	0.49486	0.28876	0.7853
C_benz1	C	0.4363	0.31244	0.78927
C_benz2	C	0.42849	0.37498	0.7916
C_benz3	C	0.47556	0.41538	0.79145
C_benz2	C	0.53246	0.39154	0.78842
C_COO	C	0.38454	0.2722	0.78722

C_COO	C	0.60534	0.30998	0.77627
O_COO2	O	0.61411	0.25622	0.75785
O_COO1	O	0.64693	0.34684	0.7864
O_COO1	O	0.33239	0.29196	0.78996
O_COO2	O	0.39239	0.21436	0.78076
N1	N	0.46288	0.47776	0.79148
N_2	N	0.5049	0.22937	0.78341
H_benz	H	0.3843	0.3929	0.79215
H_benz	H	0.569	0.42256	0.78753
In1	In	0.22573	0.69412	0.18794
C_benz1	C	0.19487	0.45629	0.35076
C_benz4	C	0.19744	0.50673	0.31036
C_benz1	C	0.19274	0.56601	0.33585
C_benz2	C	0.18982	0.57275	0.39835
C_benz3	C	0.18962	0.52355	0.43735
C_benz2	C	0.19068	0.46572	0.41219
C_COO	C	0.19375	0.62112	0.29844
C_COO	C	0.19684	0.39324	0.32906
O_COO2	O	0.21667	0.37968	0.27754
O_COO1	O	0.17735	0.35318	0.36633
O_COO1	O	0.18587	0.67214	0.32174
O_COO2	O	0.20421	0.61419	0.2411
N1	N	0.19049	0.53464	0.49996
N_2	N	0.20283	0.49749	0.25099
H_benz	H	0.18939	0.61785	0.41722
H_benz	H	0.18976	0.42737	0.44229
In1	In	0.74627	0.694	0.81214
C_benz1	C	0.77722	0.45626	0.64929
C_benz4	C	0.77465	0.50667	0.68972
C_benz1	C	0.77924	0.56597	0.66427
C_benz2	C	0.78205	0.57275	0.60176
C_benz3	C	0.78221	0.52358	0.56273
C_benz2	C	0.78124	0.46573	0.58785
C_COO	C	0.77821	0.62105	0.70171
C_COO	C	0.77538	0.39321	0.67101
O_COO2	O	0.75562	0.37961	0.72256
O_COO1	O	0.79488	0.35317	0.63371
O_COO1	O	0.78595	0.67211	0.67844
O_COO2	O	0.76788	0.61408	0.75907
N1	N	0.78118	0.53471	0.50014
N_2	N	0.76941	0.49735	0.74909
H_benz	H	0.78245	0.61786	0.58291
H_benz	H	0.78217	0.4274	0.55773
Mg1	Mg	0.21621	0.29826	0.82768

C_benz1	C	0.21007	0.54085	0.68988
C_benz4	C	0.21298	0.48325	0.71983
C_benz1	C	0.2024	0.43021	0.68484
C_benz2	C	0.19355	0.43572	0.62349
C_benz3	C	0.19421	0.4914	0.59352
C_benz2	C	0.20131	0.54377	0.62781
C_COO	C	0.20161	0.36882	0.71177
C_COO	C	0.21918	0.59679	0.72363
O_COO2	O	0.23315	0.59199	0.78029
O_COO1	O	0.21496	0.64856	0.70001
O_COO1	O	0.18163	0.32647	0.68006
O_COO2	O	0.22178	0.36134	0.76545
N1	N	0.18952	0.48666	0.53097
N_2	N	0.22456	0.47799	0.77855
H_benz	H	0.18713	0.39531	0.59679
H_benz	H	0.2018	0.58724	0.60553
Mg1	Mg	0.75562	0.29833	0.17229
C_benz1	C	0.76162	0.54087	0.31038
C_benz4	C	0.75866	0.48328	0.28041
C_benz1	C	0.76914	0.4302	0.31539
C_benz2	C	0.77792	0.43567	0.37676
C_benz3	C	0.77728	0.49135	0.40675
C_benz2	C	0.77028	0.54374	0.37247
C_COO	C	0.77007	0.36883	0.2884
C_COO	C	0.75267	0.59686	0.27664
O_COO2	O	0.73876	0.59215	0.21995
O_COO1	O	0.75698	0.64862	0.30028
O_COO1	O	0.78999	0.32644	0.32013
O_COO2	O	0.75014	0.36138	0.23462
N1	N	0.78203	0.48665	0.4693
N_2	N	0.74711	0.47808	0.22168
H_benz	H	0.78428	0.39526	0.40345
H_benz	H	0.76983	0.58721	0.39475
In1	In	0.72171	0.68397	0.19452
C_benz1	C	0.68674	0.83229	0.95043
C_benz4	C	0.68417	0.79646	0.00449
C_benz1	C	0.67736	0.82682	0.06124
C_benz2	C	0.67434	0.88937	0.06207
C_benz3	C	0.67738	0.92405	0.00991
C_benz2	C	0.68249	0.89451	0.95435
C_COO	C	0.67726	0.79566	0.12041
C_COO	C	0.69635	0.80584	0.88944
O_COO2	O	0.71556	0.75061	0.88804
O_COO1	O	0.68708	0.83759	0.8435

O_COO1	O	0.66621	0.82461	0.16754
O_COO2	O	0.69047	0.73823	0.11916
N1	N	0.67785	0.98657	0.0186
N_2	N	0.68679	0.73616	0.0016
H_benz	H	0.67117	0.91227	0.10514
H_benz	H	0.68505	0.92115	0.91354
Mg1	Mg	0.2413	0.3214	0.20415
C_benz1	C	0.27659	0.17224	0.96309
C_benz4	C	0.27236	0.20699	0.01746
C_benz1	C	0.27909	0.17605	0.07363
C_benz2	C	0.28607	0.114	0.07384
C_benz3	C	0.28819	0.0799	0.02117
C_benz2	C	0.28463	0.11021	0.96611
C_COO	C	0.27711	0.20657	0.13309
C_COO	C	0.27232	0.19969	0.90251
O_COO2	O	0.25453	0.25423	0.89613
O_COO1	O	0.28639	0.16526	0.85862
O_COO1	O	0.2883	0.17408	0.17897
O_COO2	O	0.26331	0.26261	0.13535
N1	N	0.29196	0.01754	0.02929
N_2	N	0.26331	0.26659	0.016
H_benz	H	0.28903	0.09091	0.11679
H_benz	H	0.28701	0.08449	0.9247
Mg1	Mg	0.73083	0.32119	0.79576
C_benz1	C	0.69554	0.17197	0.03679
C_benz4	C	0.69987	0.20669	0.9824
C_benz1	C	0.69304	0.17578	0.92622
C_benz2	C	0.68593	0.11374	0.92603
C_benz3	C	0.68379	0.07965	0.97871
C_benz2	C	0.68741	0.10995	0.03376
C_COO	C	0.69506	0.20627	0.86674
C_COO	C	0.69979	0.19946	0.09736
O_COO2	O	0.71782	0.2539	0.10375
O_COO1	O	0.68547	0.16511	0.14125
O_COO1	O	0.6839	0.17379	0.82085
O_COO2	O	0.70885	0.26231	0.86448
N1	N	0.67993	0.01731	0.97062
N_2	N	0.70916	0.26625	0.98394
H_benz	H	0.6829	0.09066	0.88309
H_benz	H	0.68502	0.08424	0.07517
In1	In	0.25022	0.68383	0.80567
C_benz1	C	0.28514	0.83238	0.04962
C_benz4	C	0.28784	0.79648	0.9956
C_benz1	C	0.29465	0.82682	0.93883

C_benz2	C	0.29762	0.88938	0.93796
C_benz3	C	0.29452	0.9241	0.9901
C_benz2	C	0.28936	0.89459	0.04566
C_COO	C	0.29472	0.7956	0.87969
C_COO	C	0.27544	0.80595	0.1106
O_COO2	O	0.2562	0.75073	0.11193
O_COO1	O	0.28467	0.83766	0.15657
O_COO1	O	0.30582	0.82449	0.83254
O_COO2	O	0.28145	0.73819	0.88099
N1	N	0.29407	0.98663	0.98138
N_2	N	0.28535	0.73619	0.99855
H_benz	H	0.30078	0.91224	0.89488
H_benz	H	0.28673	0.92126	0.08646
Mg1	Mg	0.67764	0.19726	0.73367
C_benz1	C	0.82776	0.95564	0.70313
C_benz4	C	0.79481	0.01093	0.70374
C_benz1	C	0.82562	0.06666	0.69524
C_benz2	C	0.88642	0.06565	0.69128
C_benz3	C	0.91906	0.01267	0.69403
C_benz2	C	0.8884	0.9578	0.69827
C_COO	C	0.79579	0.12582	0.69267
C_COO	C	0.79858	0.89496	0.70844
O_COO2	O	0.74532	0.89214	0.72675
O_COO1	O	0.82951	0.84922	0.69517
O_COO1	O	0.82896	0.17088	0.67738
O_COO2	O	0.74195	0.13088	0.70568
N1	N	0.98002	0.02145	0.69284
N_2	N	0.73664	0.00989	0.71076
H_benz	H	0.90989	0.10789	0.68693
H_benz	H	0.91277	0.91586	0.69877
Mg1	Mg	0.29455	0.19745	0.26605
C_benz1	C	0.1443	0.95575	0.29689
C_benz4	C	0.17726	0.01103	0.29622
C_benz1	C	0.14645	0.06678	0.30457
C_benz2	C	0.08565	0.06578	0.3085
C_benz3	C	0.05299	0.01279	0.30589
C_benz2	C	0.08366	0.95791	0.30175
C_COO	C	0.17634	0.12592	0.30712
C_COO	C	0.17346	0.89505	0.29166
O_COO2	O	0.22673	0.89222	0.27338
O_COO1	O	0.14254	0.8493	0.30495
O_COO1	O	0.14319	0.17097	0.32248
O_COO2	O	0.23017	0.13098	0.29405
N1	N	-0.00797	0.02157	0.30709

N_2	N	0.23544	0.01004	0.28927
H_benz	H	0.0622	0.10805	0.31273
H_benz	H	0.05927	0.91598	0.30132
Mg1	Mg	0.30904	0.80508	0.73798
C_benz1	C	0.16097	0.04538	0.70668
C_benz4	C	0.19625	0.99179	0.70651
C_benz1	C	0.16794	0.93493	0.69727
C_benz2	C	0.10729	0.93317	0.69282
C_benz3	C	0.07236	0.98474	0.69541
C_benz2	C	0.10049	0.04063	0.7007
C_COO	C	0.20025	0.87648	0.69524
C_COO	C	0.18643	0.10704	0.71333
O_COO2	O	0.24042	0.1122	0.73099
O_COO1	O	0.1532	0.15118	0.70181
O_COO1	O	0.17131	0.83047	0.67892
O_COO2	O	0.25447	0.87522	0.71124
N1	N	0.01153	0.97452	0.69353
N_2	N	0.25441	0.99476	0.71354
H_benz	H	0.08576	0.88985	0.68824
H_benz	H	0.07429	0.08129	0.70154
Mg1	Mg	0.66298	0.8053	0.26218
C_benz1	C	0.811	0.04545	0.29335
C_benz4	C	0.77576	0.99184	0.29355
C_benz1	C	0.80411	0.93502	0.30286
C_benz2	C	0.86476	0.93328	0.3073
C_benz3	C	0.89966	0.98486	0.30466
C_benz2	C	0.87149	0.04073	0.29929
C_COO	C	0.77173	0.87663	0.30491
C_COO	C	0.78553	0.10712	0.28669
O_COO2	O	0.73159	0.11228	0.2689
O_COO1	O	0.81872	0.15125	0.29837
O_COO1	O	0.80064	0.83063	0.32126
O_COO2	O	0.7175	0.87542	0.28891
N1	N	0.9605	0.97465	0.30654
N_2	N	0.71758	0.99455	0.28652
H_benz	H	0.88632	0.88998	0.31195
H_benz	H	0.89766	0.08141	0.29843
Mg1	Mg	0.18832	0.74077	0.68498
C_benz1	C	0.94336	0.71139	0.82895
C_benz4	C	-0.00335	0.71526	0.79401
C_benz1	C	0.05186	0.70786	0.82443
C_benz2	C	0.05178	0.70235	0.88698
C_benz3	C	0.00072	0.70215	0.9215
C_benz2	C	0.94694	0.70498	0.89115

C_COO	C	0.11018	0.70756	0.79326
C_COO	C	0.88339	0.71552	0.80128
O_COO2	O	0.87706	0.7325	0.74694
O_COO1	O	0.84037	0.70184	0.83654
O_COO1	O	0.15422	0.69379	0.82647
O_COO2	O	0.11407	0.72126	0.73737
N1	N	0.00901	0.70032	0.98432
N_2	N	-0.00526	0.72484	0.73442
H_benz	H	0.09334	0.69905	0.91026
H_benz	H	0.90703	0.70331	0.91741
In1	In	0.17363	0.26361	0.32784
C_benz1	C	0.94273	0.29846	0.16789
C_benz4	C	-0.00524	0.29717	0.20425
C_benz1	C	0.05024	0.3089	0.17572
C_benz2	C	0.0518	0.31659	0.11338
C_benz3	C	0.00153	0.31474	0.07788
C_benz2	C	0.94736	0.30738	0.10646
C_COO	C	0.10672	0.30951	0.20885
C_COO	C	0.88274	0.28941	0.19312
O_COO2	O	0.87627	0.26747	0.24597
O_COO1	O	0.84032	0.30396	0.15869
O_COO1	O	0.15338	0.3239	0.18177
O_COO2	O	0.10455	0.29418	0.26541
N1	N	0.00935	0.31773	0.01534
N_2	N	0.9904	0.2863	0.2634
H_benz	H	0.09367	0.32278	0.09126
H_benz	H	0.90819	0.30727	0.07907
Mg1	Mg	0.7836	0.74084	0.31525
C_benz1	C	0.0286	0.71144	0.17129
C_benz4	C	0.97534	0.71531	0.20627
C_benz1	C	0.92013	0.70786	0.1759
C_benz2	C	0.92016	0.70235	0.11335
C_benz3	C	0.97119	0.70215	0.07878
C_benz2	C	0.02499	0.70501	0.10909
C_COO	C	0.86181	0.70757	0.20708
C_COO	C	0.08858	0.71559	0.19893
O_COO2	O	0.0949	0.73264	0.25324
O_COO1	O	0.1316	0.70191	0.16368
O_COO1	O	0.81782	0.69377	0.17383
O_COO2	O	0.85786	0.7213	0.26296
N1	N	0.96286	0.70032	0.01598
N_2	N	0.97731	0.72486	0.26586
H_benz	H	0.87857	0.69902	0.09012
H_benz	H	0.06488	0.70332	0.08282

In1	In	0.79845	0.26352	0.67195
C_benz1	C	0.0292	0.2978	0.83232
C_benz4	C	0.97726	0.29632	0.7959
C_benz1	C	0.92179	0.30823	0.82432
C_benz2	C	0.92012	0.31613	0.88664
C_benz3	C	0.97035	0.31441	0.92222
C_benz2	C	0.02453	0.30693	0.89373
C_COO	C	0.86535	0.30903	0.7911
C_COO	C	0.0892	0.28894	0.80706
O_COO2	O	0.09571	0.2671	0.75417
O_COO1	O	0.1316	0.30366	0.84146
O_COO1	O	0.81873	0.32356	0.81818
O_COO2	O	0.86748	0.29371	0.73454
N1	N	0.96246	0.31763	0.98472
N_2	N	-0.01823	0.28508	0.73682
H_benz	H	0.87819	0.32241	0.90862
H_benz	H	0.06368	0.30692	0.92115
O_OH	O	0.2105	0.22737	0.77783
O_OH	O	0.75905	0.77578	0.76339
O_OH	O	0.76155	0.22739	0.22206
O_OH	O	0.21301	0.77581	0.23682
O_OH	O	0.73752	0.76427	0.24416
O_OH	O	0.22601	0.24812	0.25028
O_OH	O	0.74615	0.24798	0.74953
O_OH	O	0.2345	0.76411	0.75602
H_OH	H	0.21202	0.79202	0.78034
H_OH	H	0.18903	0.80202	0.21196
H_OH	H	0.20341	0.22242	0.22359
H_OH	H	0.78278	0.19504	0.20235
H_OH	H	0.76889	0.22233	0.77615
H_OH	H	0.78305	0.80196	0.78827
H_OH	H	0.76008	0.79217	0.21993
H_OH	H	0.18937	0.19492	0.79747
H_2	H	0.4591	0.78142	0.76262
H_2	H	0.53747	0.78284	0.76678
H_2	H	0.46972	0.2016	0.78124
H_2	H	0.5466	0.21687	0.77403
H_2	H	0.2112	0.45486	0.23738
H_2	H	0.20658	0.53416	0.22415
H_2	H	0.2297	0.43521	0.79401
H_2	H	0.23331	0.51577	0.8024
H_2	H	0.50215	0.20181	0.21858
H_2	H	0.42532	0.21737	0.22577
H_2	H	0.5132	0.78147	0.23767

H_2	H	0.43484	0.7832	0.23346
H_2	H	0.76113	0.4547	0.76268
H_2	H	0.76565	0.53398	0.77599
H_2	H	0.7421	0.43532	0.20614
H_2	H	0.73854	0.51591	0.19784
H_2	H	0.2063	0.2282	0.47394
H_2	H	0.20673	0.22502	0.55481
H_2	H	0.76482	0.22547	0.44436
H_2	H	0.76572	0.22864	0.52523
H_2	H	0.7615	0.75026	0.46465
H_2	H	0.76642	0.76238	0.54496
H_2	H	0.20571	0.76246	0.45475
H_2	H	0.21029	0.75029	0.53507
H_2	H	0.28334	0.71375	0.95885
H_2	H	0.27421	0.71816	1.03883
H_2	H	0.27608	0.95484	0.71579
H_2	H	0.27164	1.03555	0.72358
H_2	H	0.03337	0.72953	0.71245
H_2	H	-0.04487	0.73391	0.71602
H_2	H	-0.056	0.28259	0.71316
H_2	H	0.0219	0.27278	0.7215
H_2	H	0.25354	-0.03067	0.27974
H_2	H	0.25632	0.05021	0.28681
H_2	H	0.2554	0.28566	-0.02458
H_2	H	0.25913	0.28756	0.05649
H_2	H	0.95037	0.27392	0.27893
H_2	H	1.02823	0.28382	0.28697
H_2	H	1.01694	0.73392	0.28424
H_2	H	0.9387	0.72953	0.28787
H_2	H	0.69606	0.95455	0.2843
H_2	H	0.70018	1.03525	0.27639
H_2	H	0.69793	0.7181	-0.03866
H_2	H	0.68884	0.71375	0.0413
H_2	H	0.71858	-0.03082	0.72039
H_2	H	0.71571	0.05003	0.71315
H_2	H	0.71339	0.28724	0.94346
H_2	H	0.71723	0.28522	1.02453

Table S2. LJ potential parameters for the atoms of CPM-200-In/Mg and CPM-200-In/Mg-X

Materials	Atom	ε/k^b (K)	σ (Å)
CPM-200-In/Mg	C_COO	47.3	4.0
	O_COO_1	35.0	3.22

	O_COO_2	35.0	3.22
	C_1	48.0	3.47299
	C_2 (H)	69.4362	4.43
	C_3	48.0	3.47299
	N_1	38.949[a]	3.6621[a]
	In	301.428	3.97608
	Mg	55.8574	2.69141
	O_OH	35.0	3.22
	H_OH	7.64893	2.84642
	H_Benz	none	
-N	N_2	28.0[b]	3.45[b]
-F	C_4	48.0	3.47299
	F_1	36.4834	3.0932
-OH	C_4	48.0	3.47299
	O_2	35.0	3.22
	H_2	7.64893	2.84642
$-NH_2$	N_2	111.0[b]	3.42[b]
	C_4	48.0	3.47299
	H_2	none	

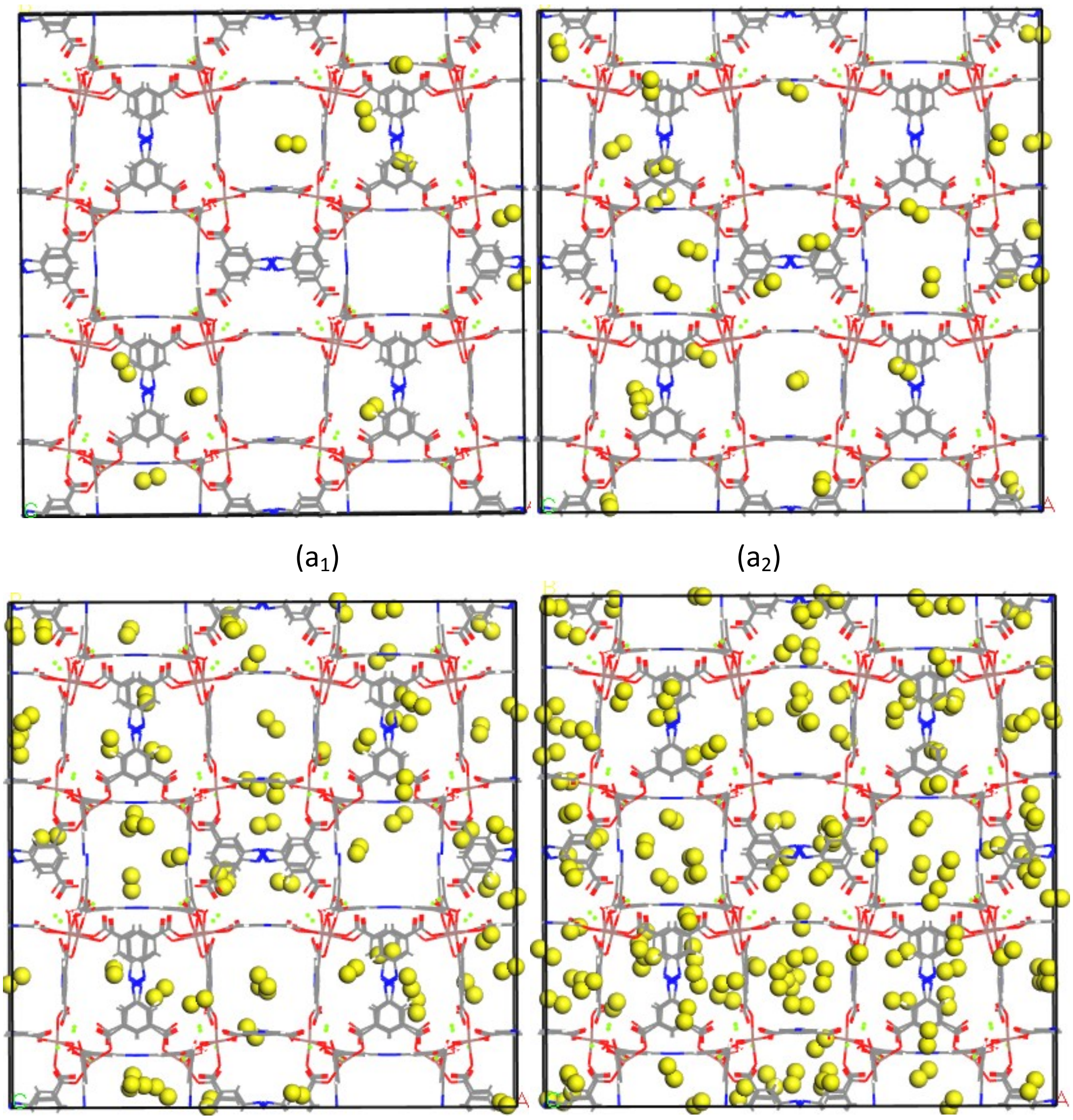
[a]The data are from Dreiding force field, [b]The data are from TraPPE force field

Table S3. LJ Potential parameters and partial charges for the adsorbates

Adsorbates	Site	ε/k^b (K)	σ (Å)	q (e)	Reference
CH_4	CH_4	148.0	3.73	0.00	TraPPE[1]
CO_2	C	27.0	2.8	0.70	TraPPE[1]
	O	79.0	3.05	-0.35	
C_2H_2	C	60.0	3.55	-0.23	TraPPE[1]
	H	15.0965	2.42	0.23	OPLS-AA[2]
H_2	H	0	0	0	(3-4)
	COM	36.7	2.958	0	
N_2	N	36	3.31	-0.482	(5)
	COM	0	0	0.964	
HCN	H	15.0965	2.42	0.202	OPLS-AA[2]
	C	60.0	3.55	0.131	TraPPE[1]
	N	60.0	2.95	-0.333	TraPPE[1]
HCHO	H	7.5482	2.42	0	OPLS-AA[2]
	C	52.838	3.75	0.45	
	O	105.676	2.96	-0.45	
C_2H_6	CH_3	98.0	3.75	0	TraPPE[1]
C_3H_8	CH_3	98.0	3.75	0	TraPPE[1]
	CH_2	46.0	3.95	0	
C_2H_4	CH_2	85.0	3.675	0	TraPPE[1]
C_2H_3Cl	C (H_2)	85.0	3.675	-0.324	TraPPE[1]
	C (H)	47.0	3.73	-0.05	
	H (CH_2)	0	0	0.177	
	H (CH)	0	0	0.152	
	Cl	149.0	3.42	-0.107	
$C_2H_2Cl_2$	C (H_2)	85.0	3.675	-0.302	TraPPE[1]
	C	22.0	3.85	0.082	
	Cl	149.0	3.42	-0.056	
	H	0	0	0.166	

Adsorbates	Site	ε/k[b] (K)	σ (Å)	q (e)	Reference
$CHCl_3$	C	10.0	4.68	-0.133	TraPPE[1]
	Cl	149.0	3.42	-0.032	
	H	0	0	0.229	
CH_2Cl_2	C	46.0	3.95	-0.132	TraPPE[1]
	Cl	149.0	3.42	-0.104	
	H	0	0	0.170	
H_2S	S	232	3.72	-0.36	TraPPE[1]
	H	0	0	0.18	
NO	N	38.9490	3.6621	-0.011	DREIDING[6]
	O	48.1579	3.4046	0.011	
CO	C	39.89	3.385	0.007	(7)
	O	61.57	2.885	-0.007	
NH_3	N	185.0	3.42	0	TraPPE[1]
	H	0	0	0.410	
	COM	0	0	-1.23	
SO_2	S	154.4	3.585	0.471	(8)
	O	62.3	2.993	0.236	

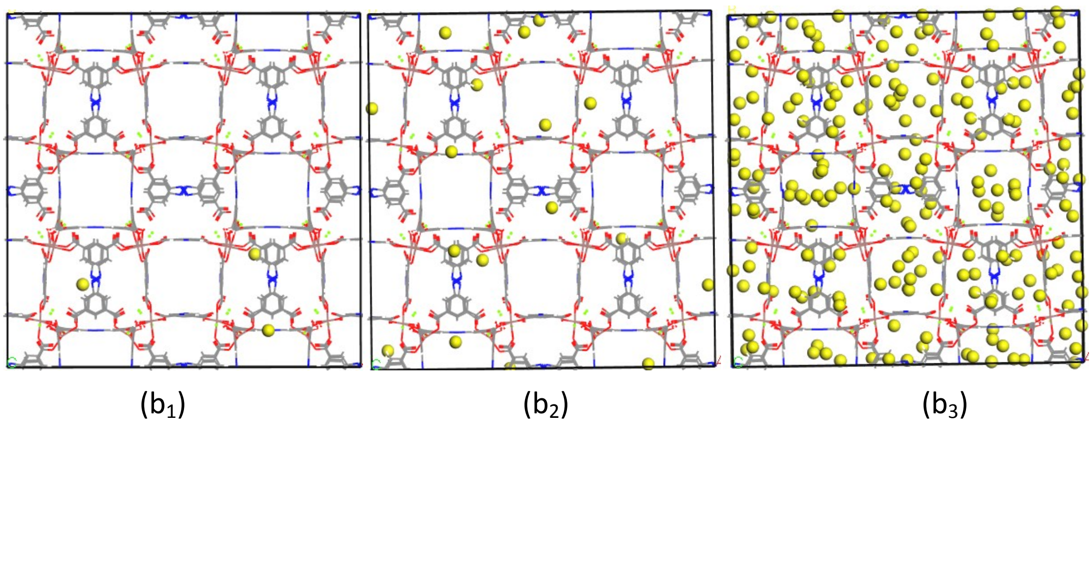
Fig. S1a



(a$_1$) (a$_2$)

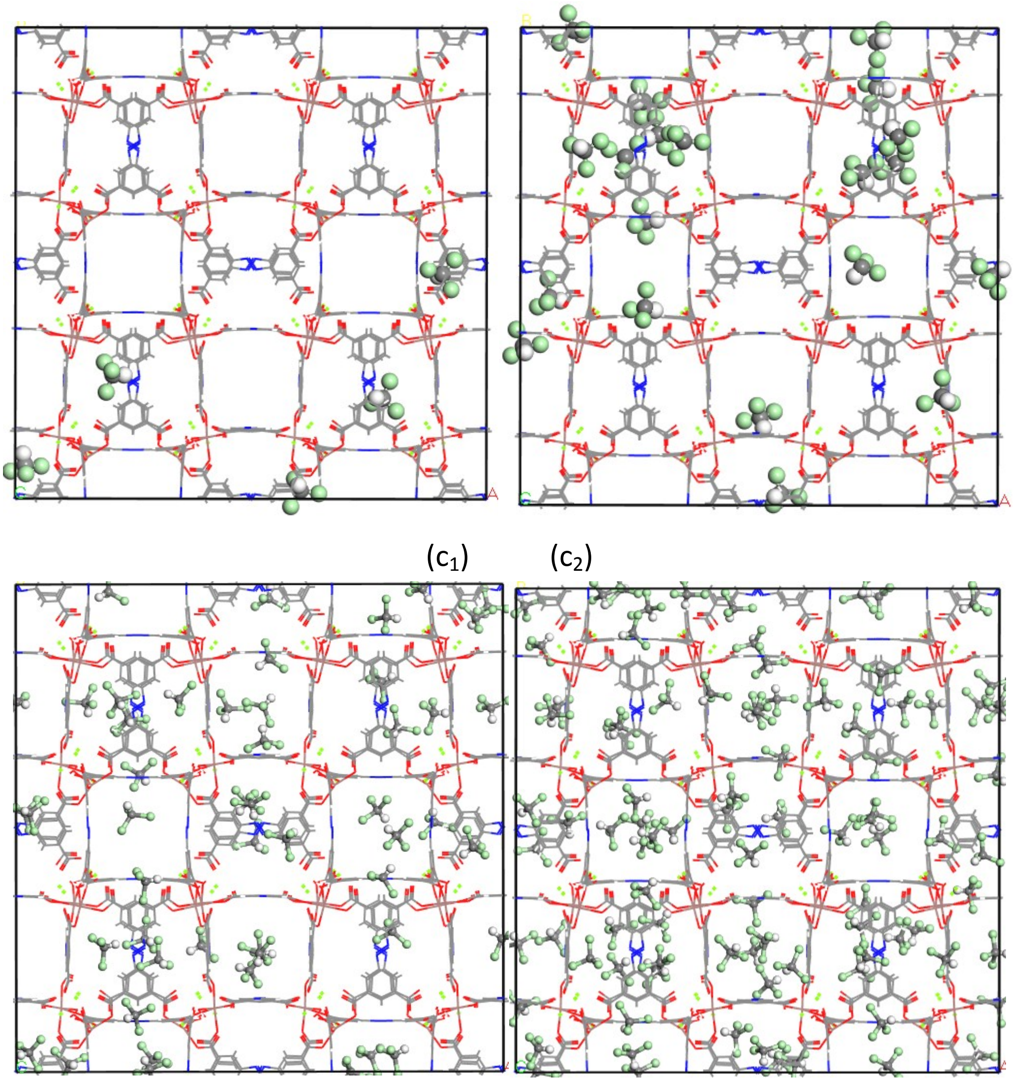
(a$_3$) (a$_4$)

Fig. S1b



(b$_1$) (b$_2$) (b$_3$)

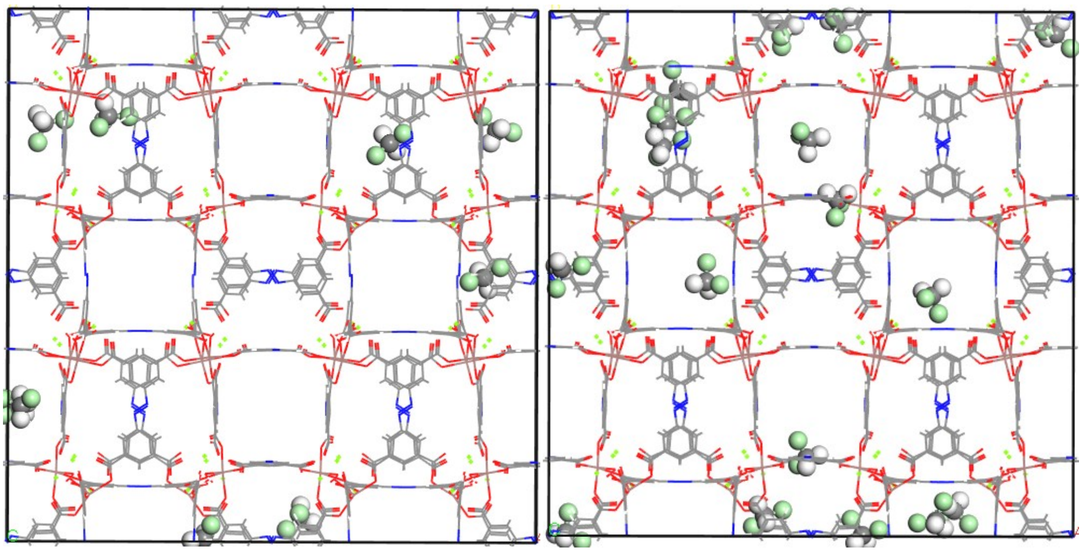
Fig. S1c



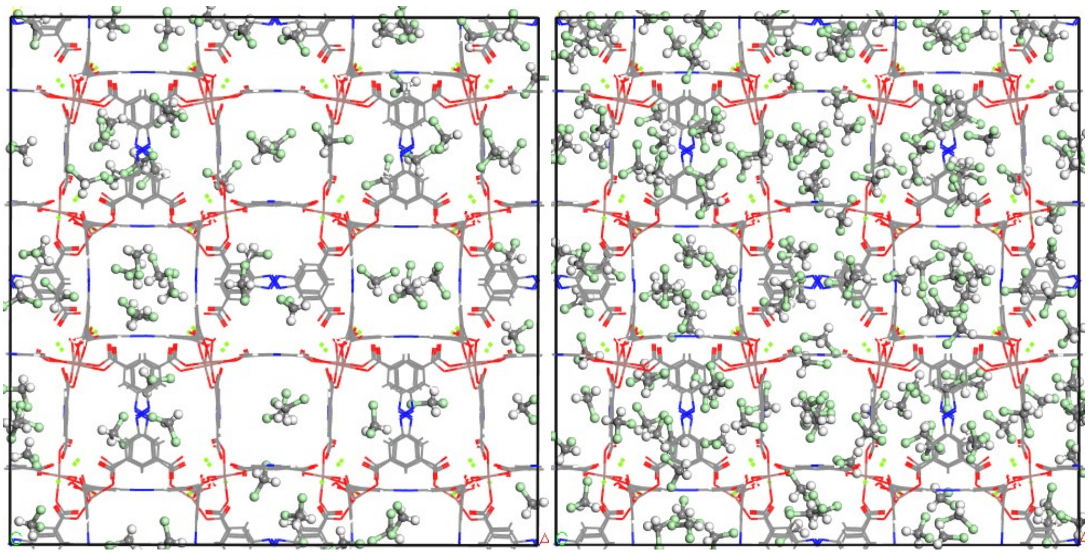
(c_1) (c_2)

(c_3) (c_4)

Fig. S1d



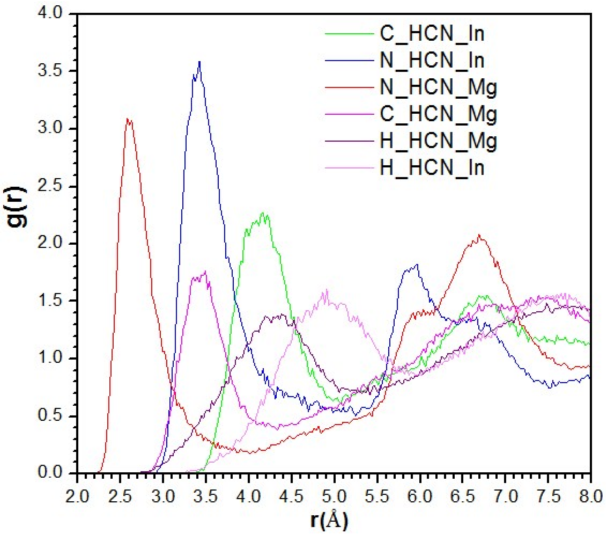
(d$_1$) (d$_2$)



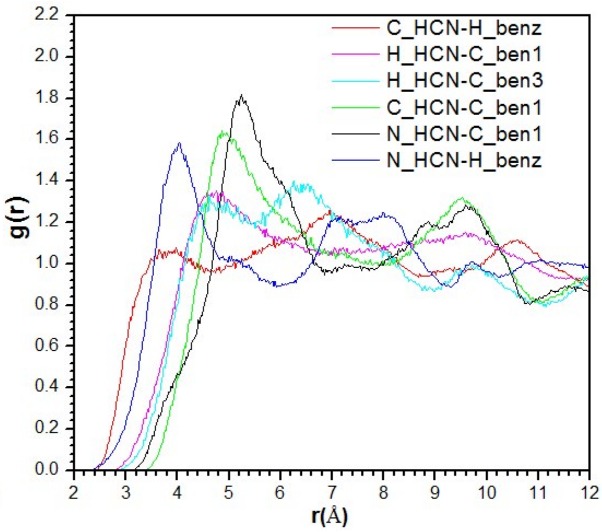
(d$_3$) (d$_4$)

Fig. S1 The snapshots of C_2H_4 adsorbed in framework at 5000 (a$_1$), 13333 (a$_2$), 40000 (a$_3$) and 100000 (a$_4$) Pa respectively;the snapshots of CH_4 adsorbed in framework at 200 Torr (b$_1$), 600 Torr (b$_2$) and 4MPa (b$_3$) respectively;the snapshots of $CHCl_3$ adsorbed in framework at 10 (c$_1$), 40 (c$_2$), 80 (c$_3$) and 300 (c$_4$) Pa respectively;the snapshots of CH_2Cl_2 adsorbed in framework at 100 (d$_1$), 200 (d$_2$), 750 (d$_3$) and 13333 (d$_4$) Pa respectively

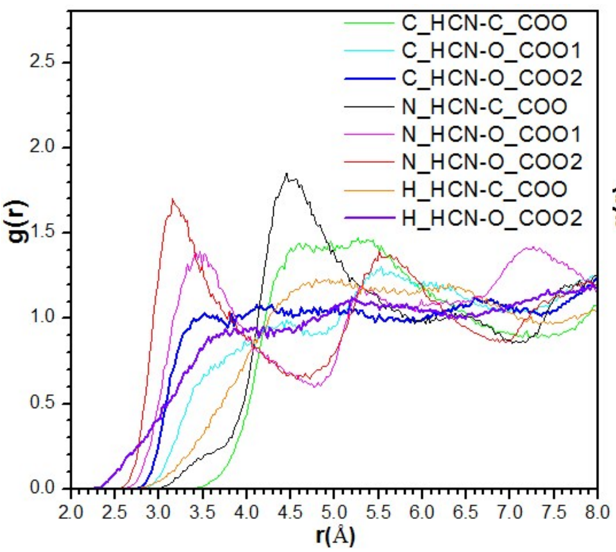
Fig. S2a



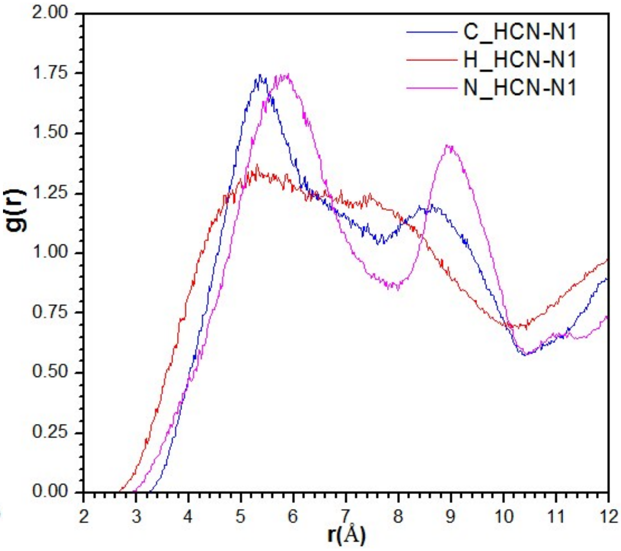
(a_1)



(a_2)

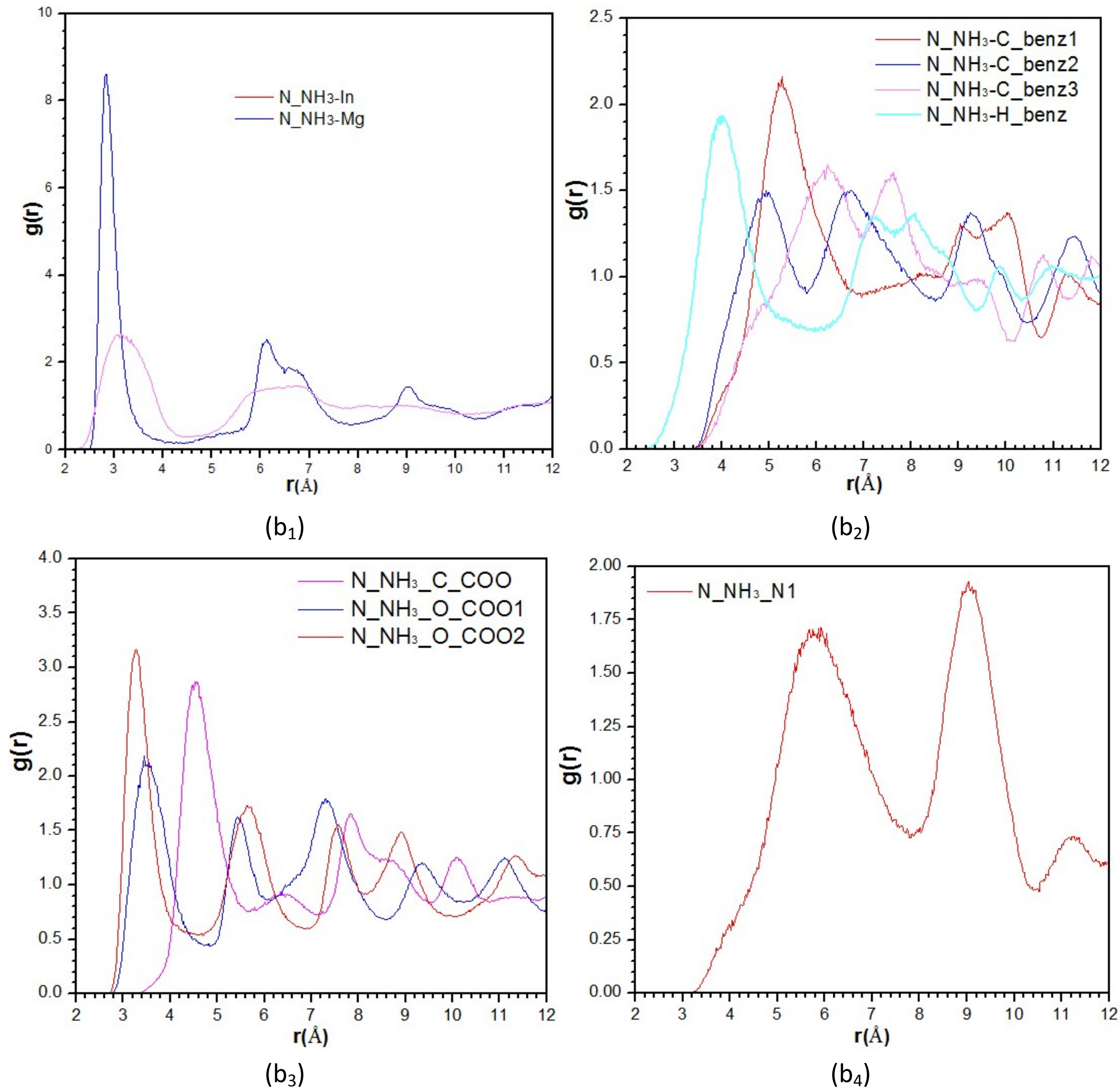


(a_3)



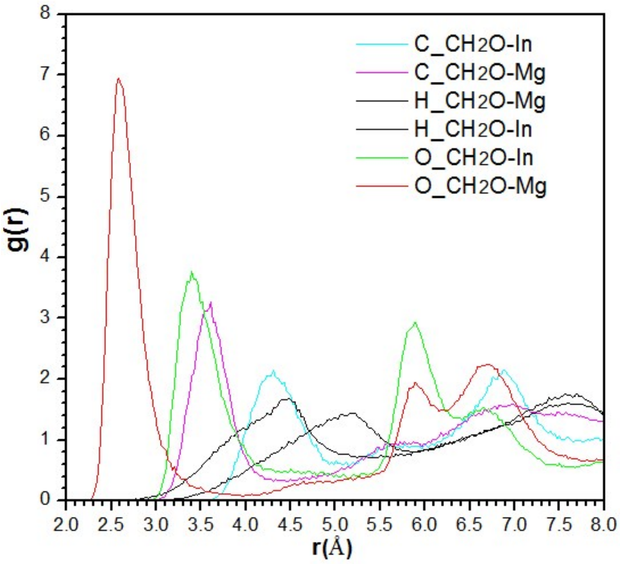
(a_4)

Fig. S2b

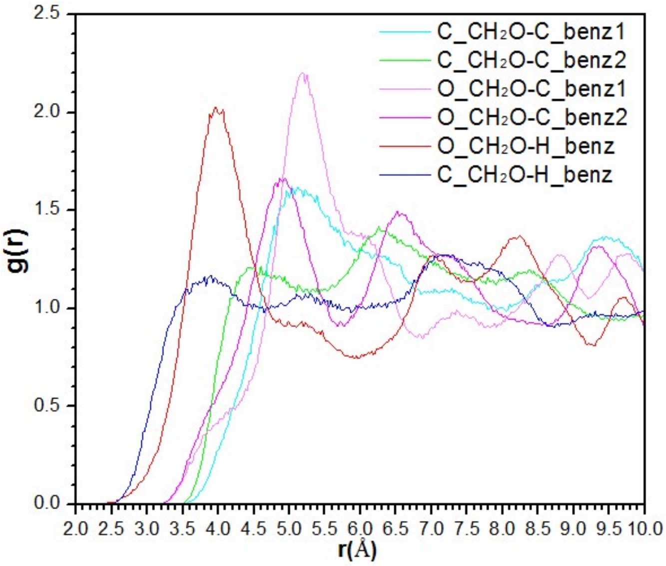


N_NH3-In
N_NH3-Mg
g(r)
r(Å)
(b$_1$)
N_NH3-C_benz1
N_NH3-C_benz2
N_NH3-C_benz3
N_NH3-H_benz
g(r)
r(Å)
(b$_2$)
N_NH3_C_COO
N_NH3_O_COO1
N_NH3_O_COO2
g(r)
r(Å)
(b$_3$)
N_NH3_N1
g(r)
r(Å)
(b$_4$)

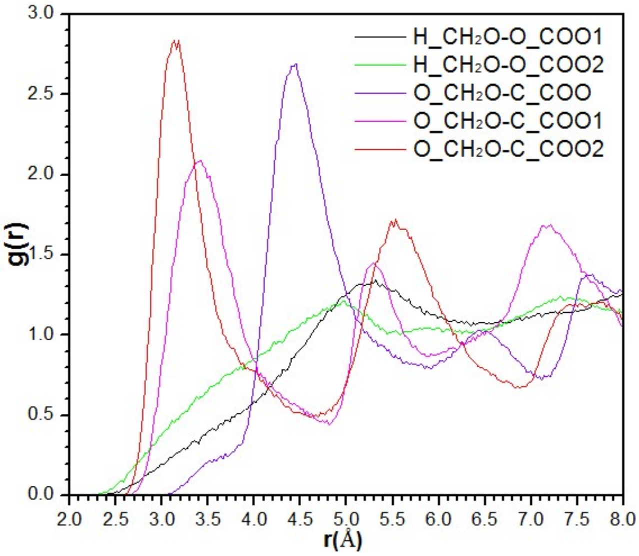
Fig. S2c



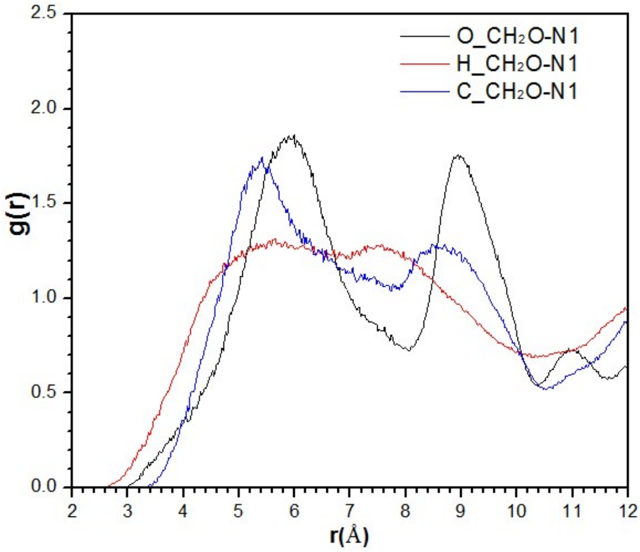
(c$_1$)



(c$_2$)

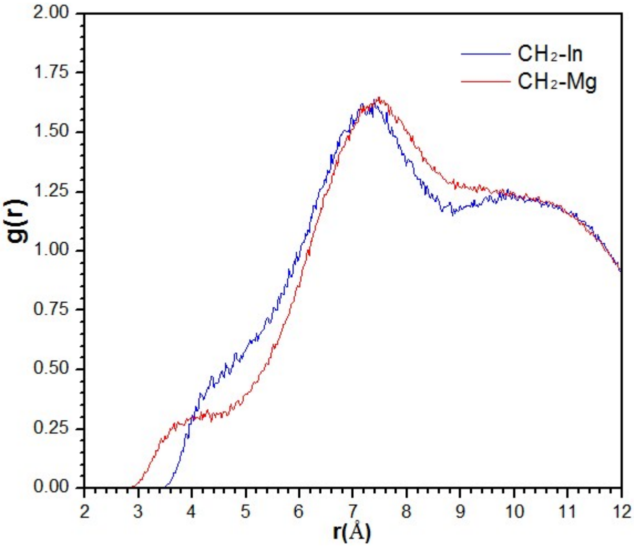


(c$_3$)

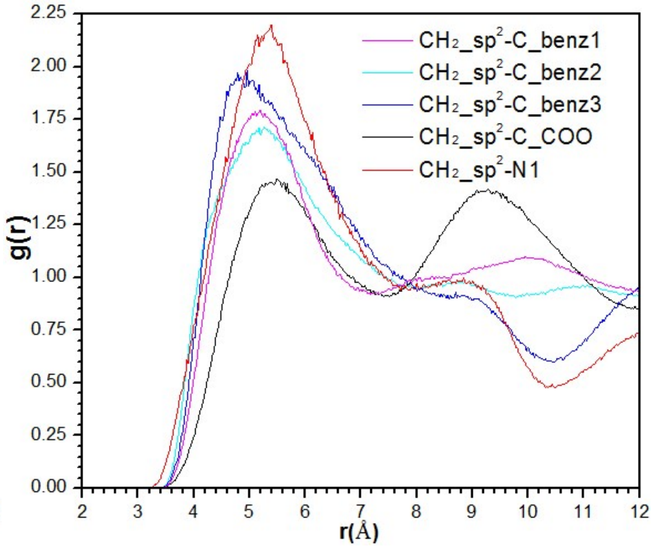


(c$_4$)

Fig. S2d

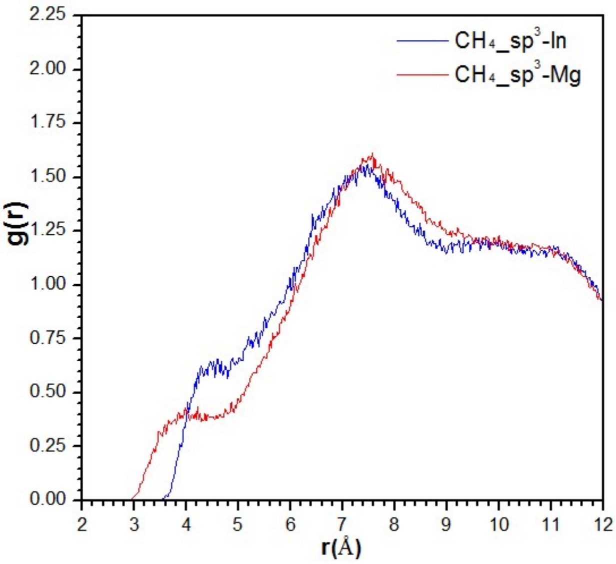


(d$_1$)

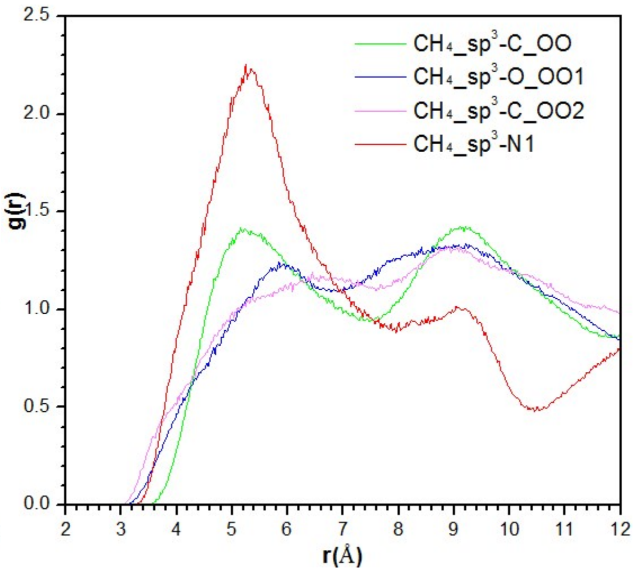


(d$_2$)

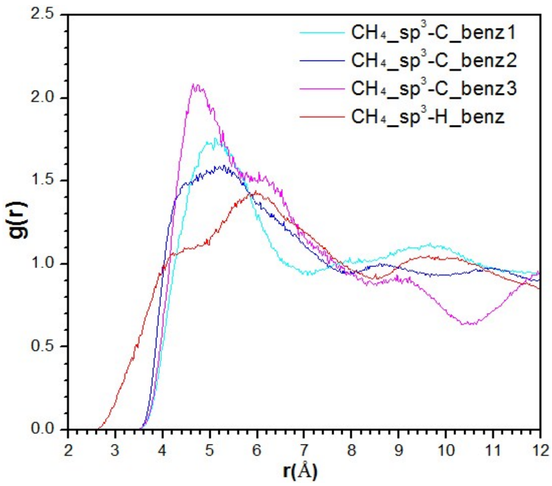
Fig. S2e



(e$_1$)

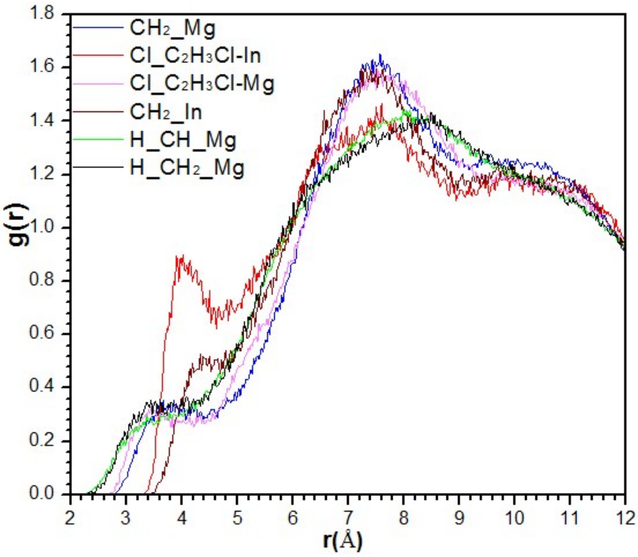


(e$_2$)

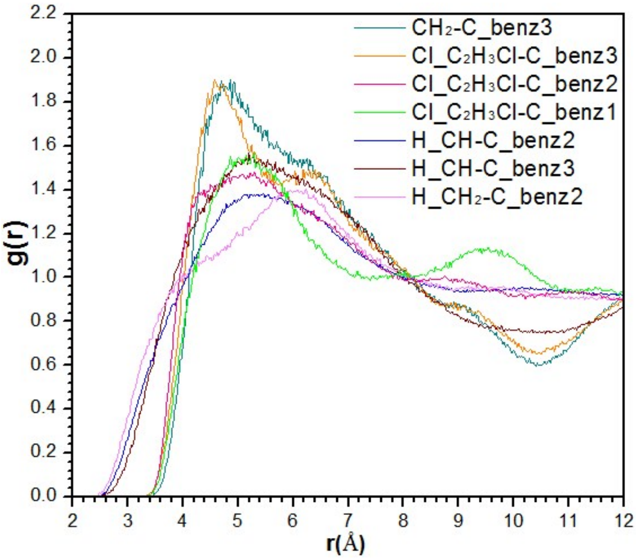


(e$_3$)

Fig. S2f



(f_1)



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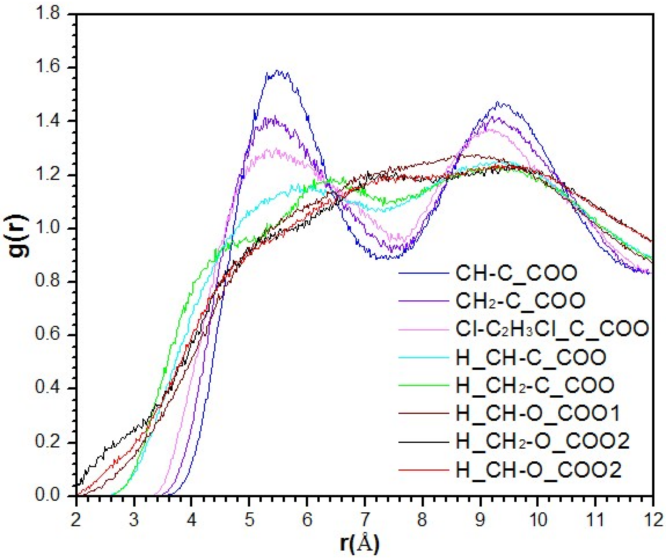

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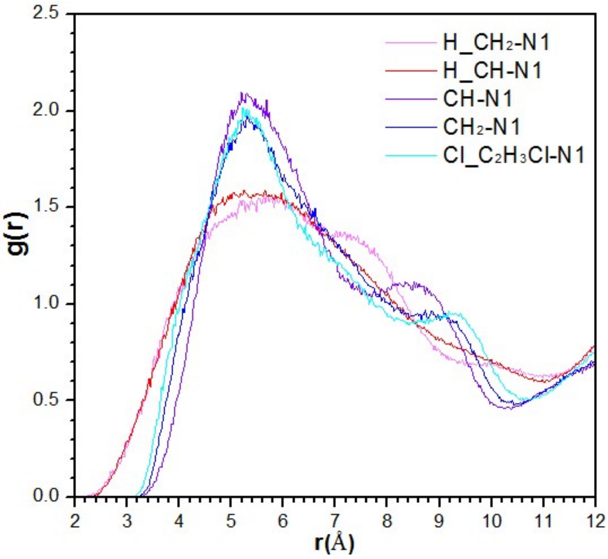
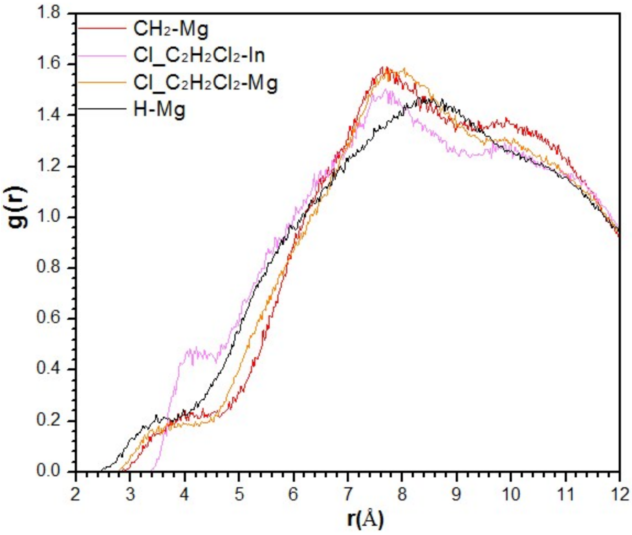
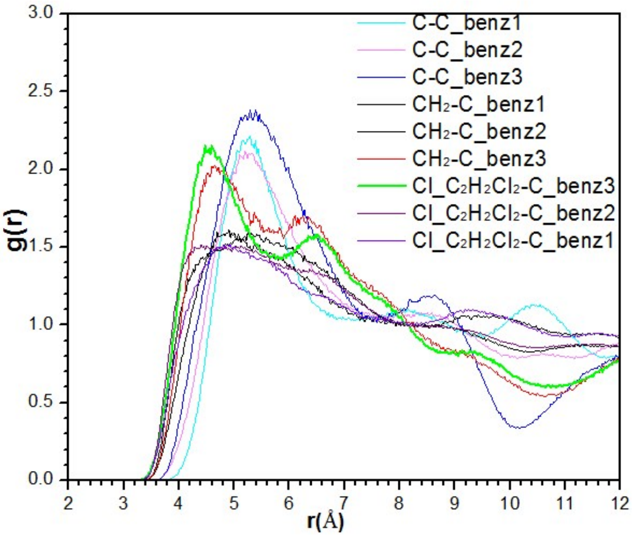


(f_4)

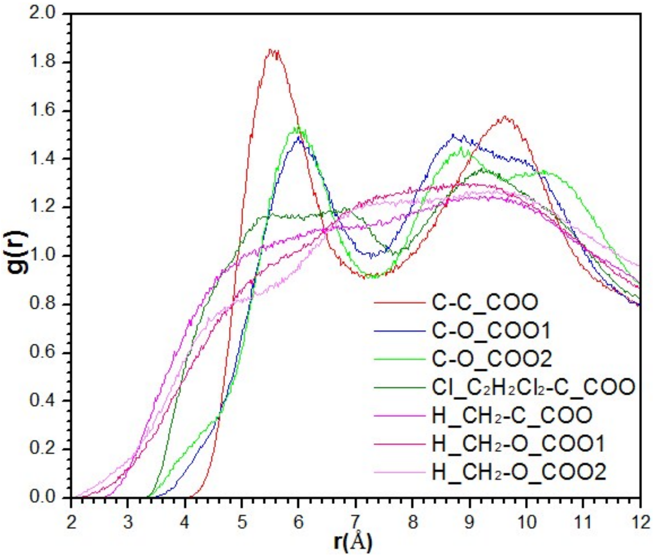
Fig. S2g



(g$_1$)



(g$_2$)



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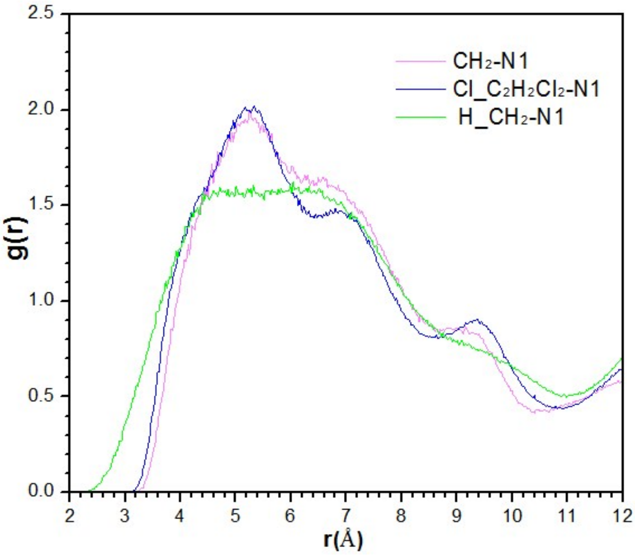
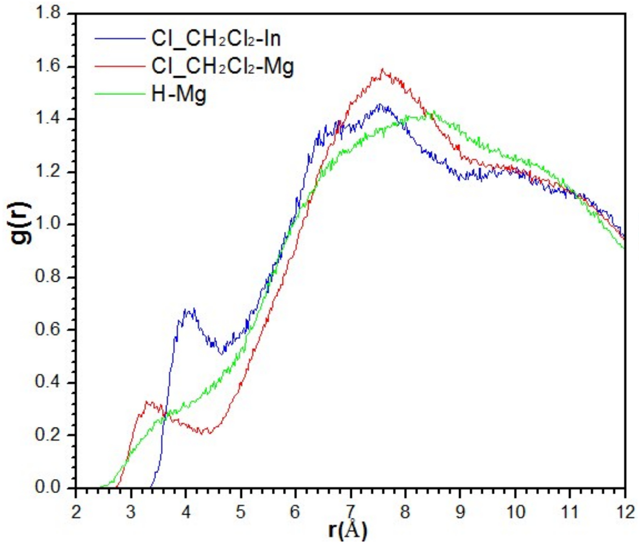
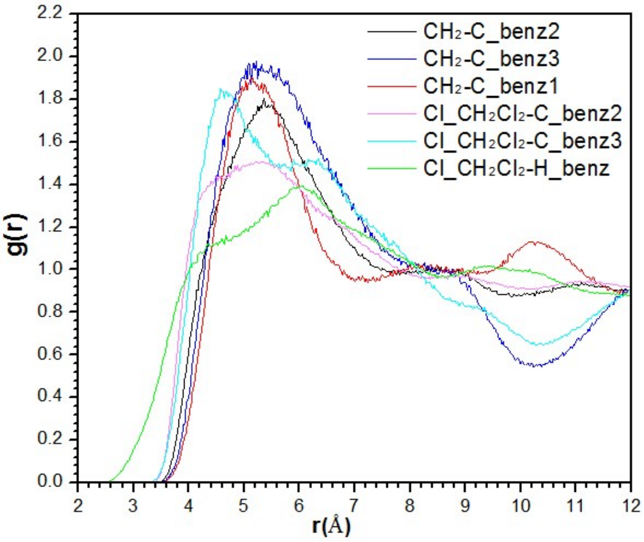


(g$_4$)

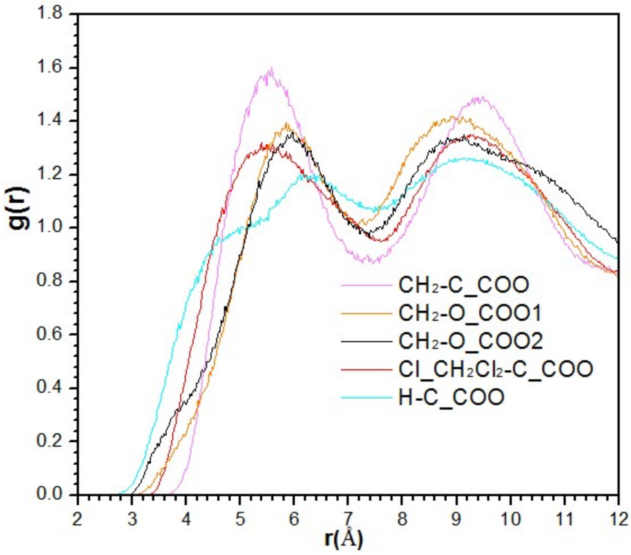
Fig. S2h



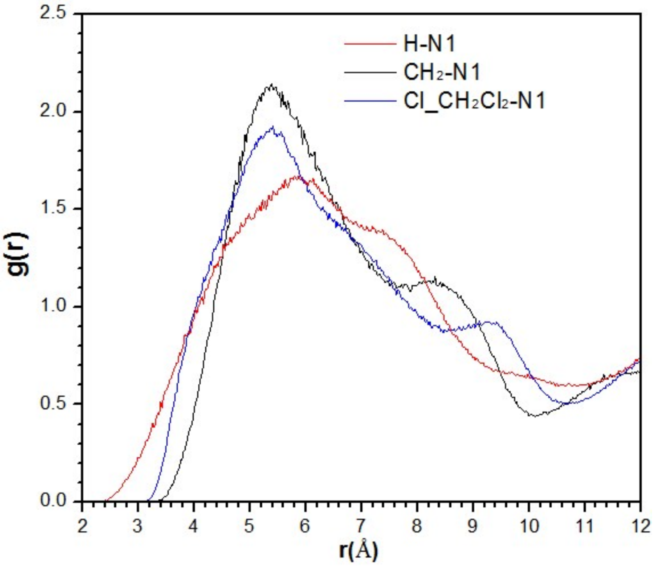
(h$_1$)



(h$_2$)

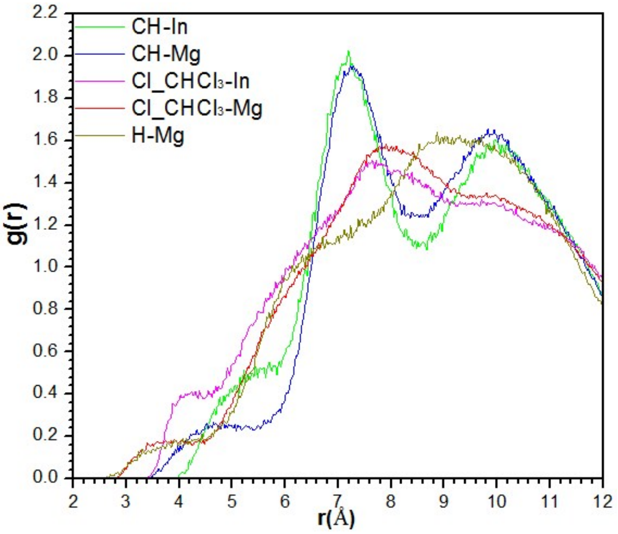


(h$_3$)

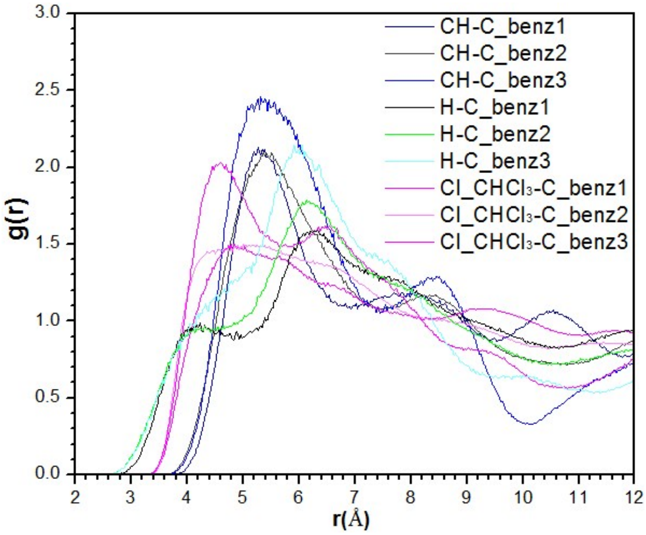


(h$_4$)

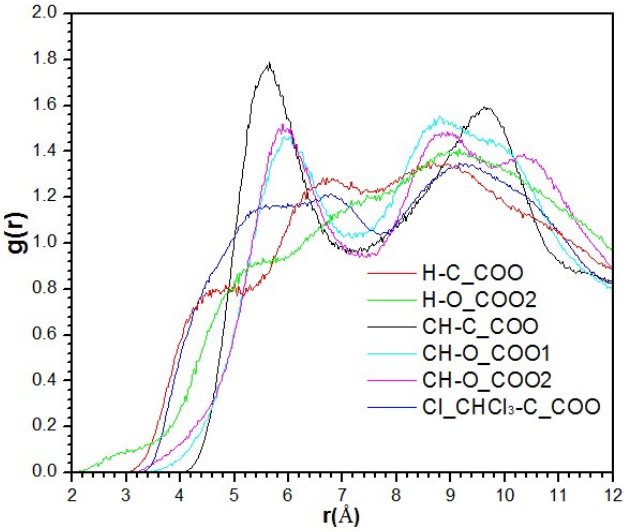
Fig. S2i



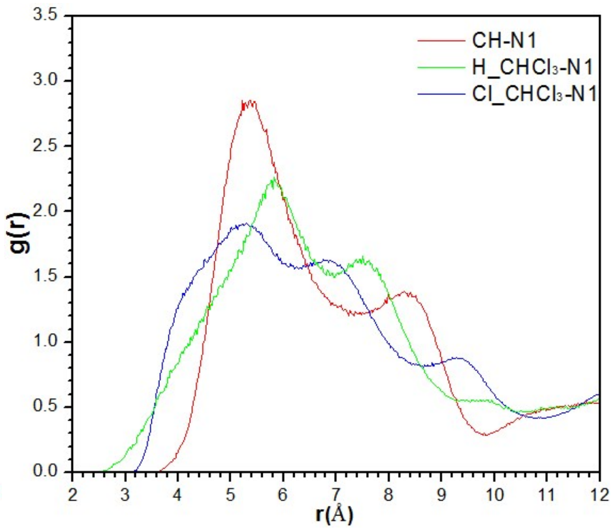
(i$_1$)



(i$_2$)



(i$_3$)



(i$_4$)

Fig.S2 Radial distribution functions g(r) computed between the harmful gases (HCN (a), NH_3 (b), HCHO (c), C_2H_4 (d), CH_4 (e), C_2H_3Cl (f), $C_2H_2Cl_2$ (g), CH_2Cl_2 (h)and$CHCl_3$ (i)) atoms and the various framework atoms at 298 K

Fig. S3

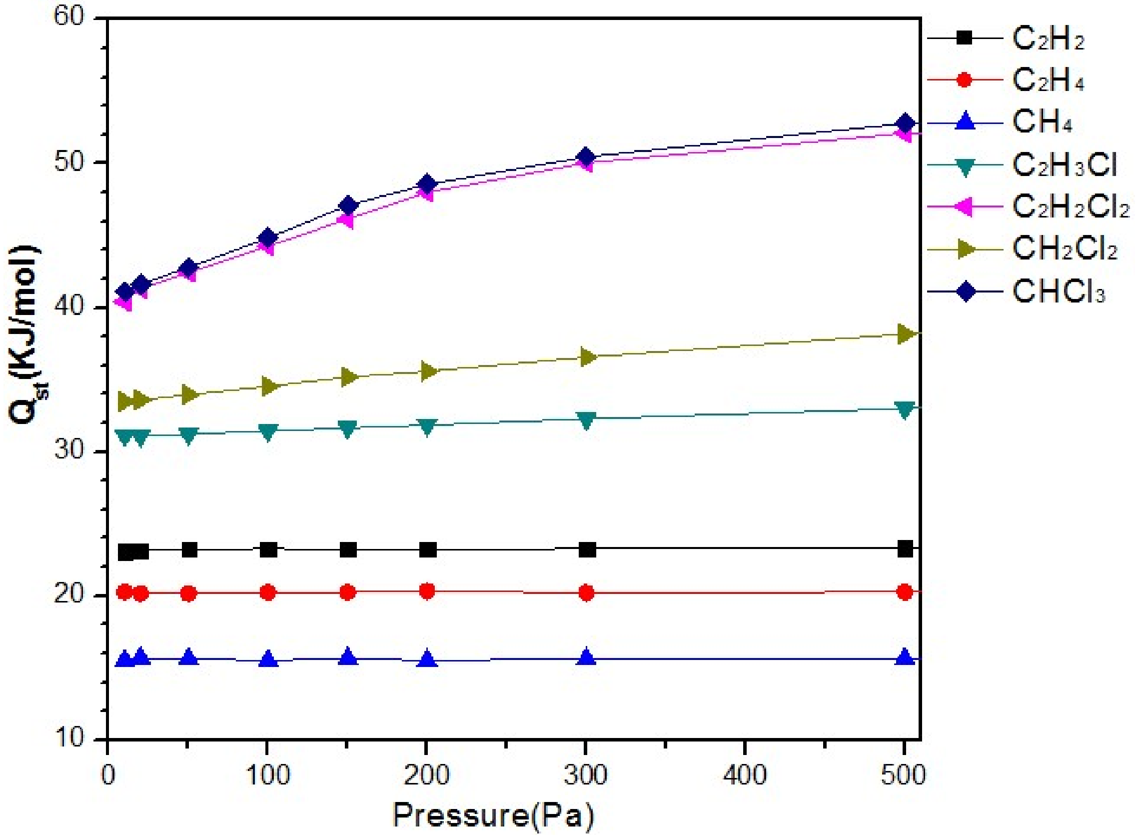


Fig.S3 Isosteric heats of C_2H_2, C_2H_4, CH_4, C_2H_3Cl, $C_2H_2Cl_2$, CH_2Cl_2 and $CHCl_3$ adsorbed inCPM-200-In/Mg at 298 K

Fig. S4

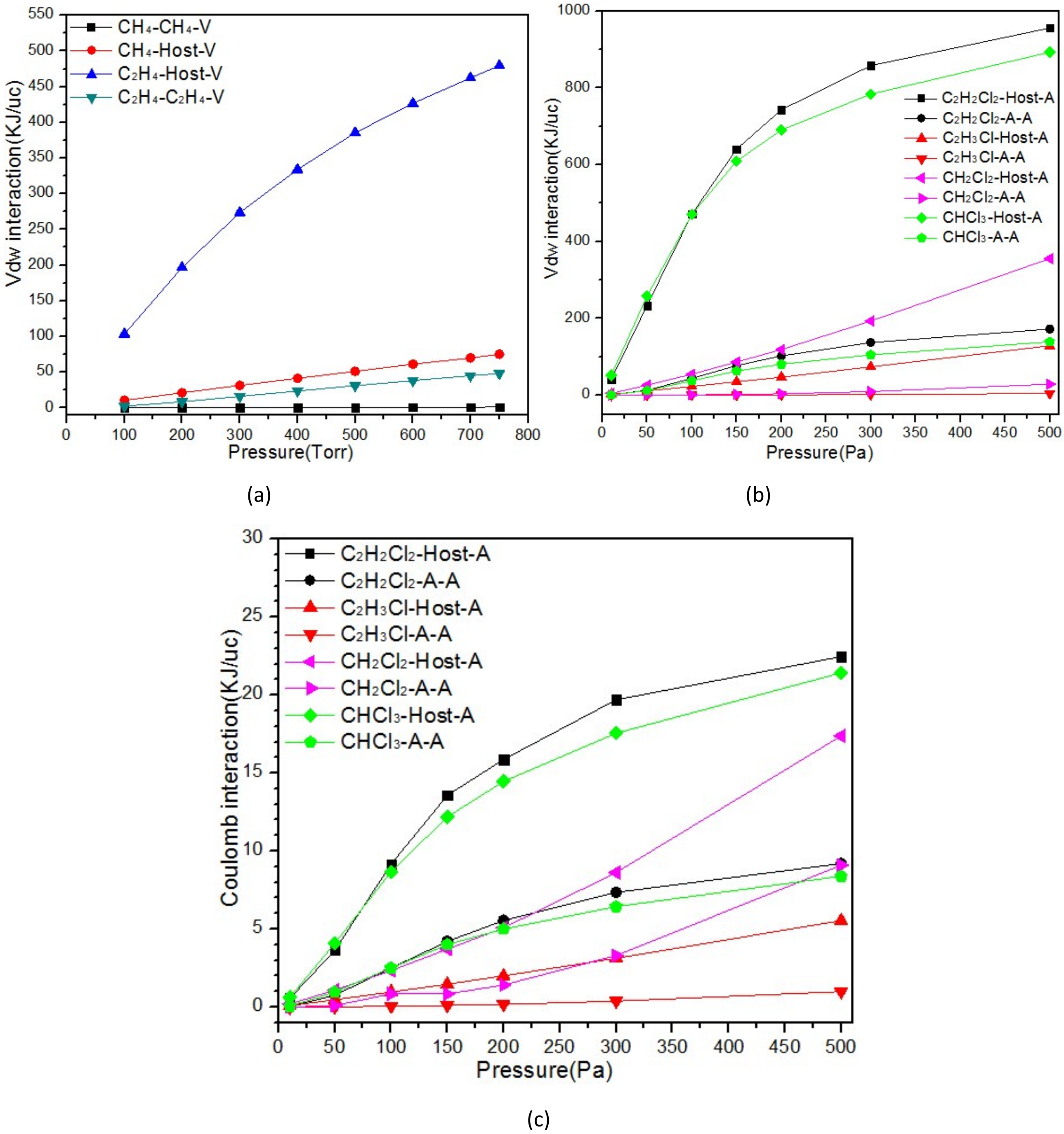
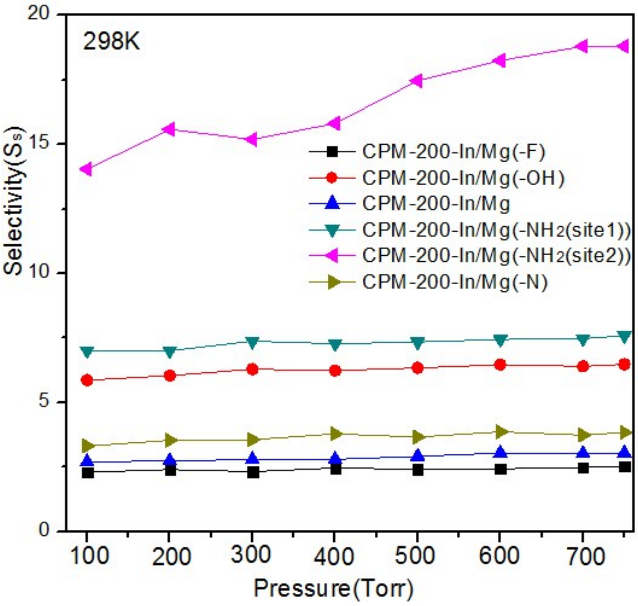
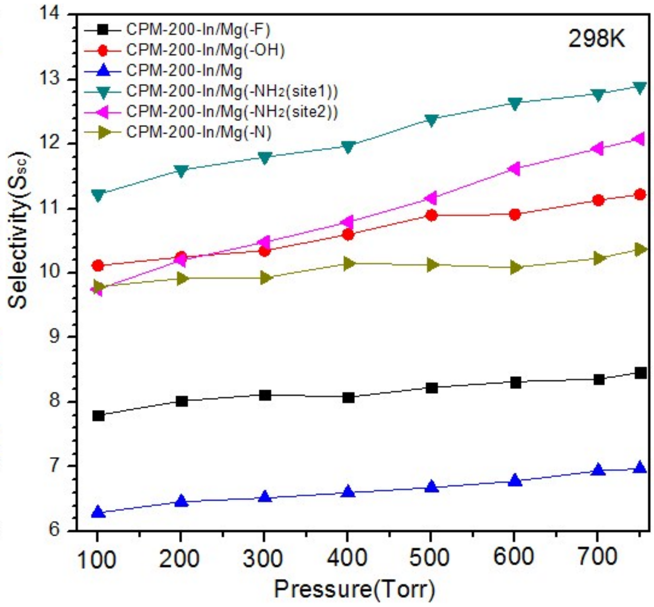


Fig.S4 The Vdw(a, b) and Coulomb(c) interactions between the host and adsorbate or among adsorbates respectively at 298 K

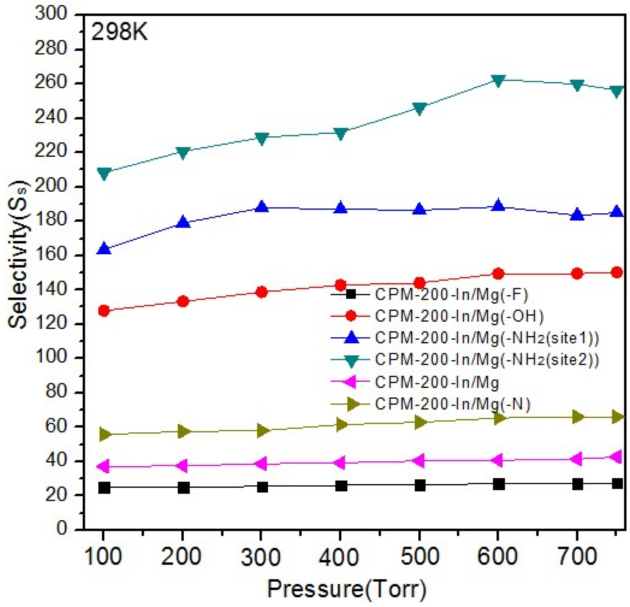
Fig. S5



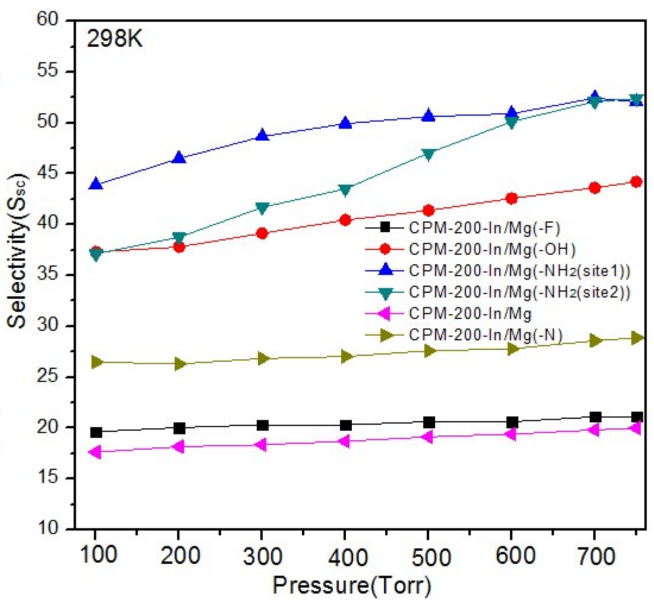
(a)



(b)



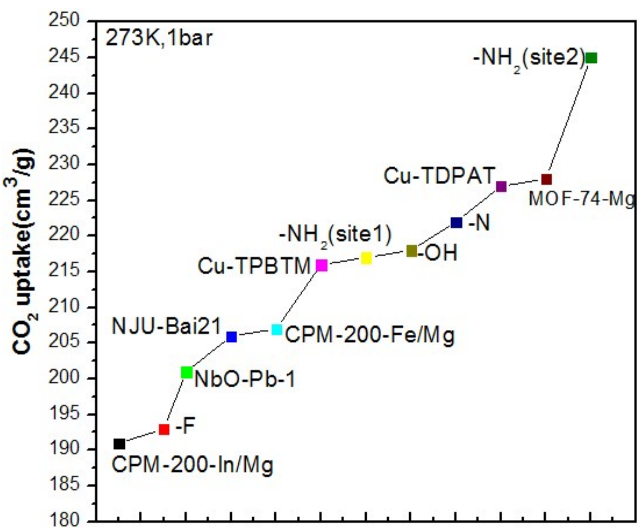
(c)



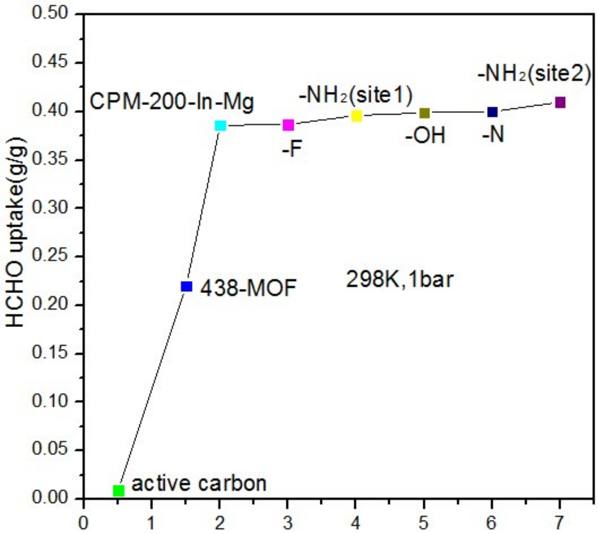
(d)

Fig.S5 Adsorption selectivities of MOFs in CO_2-H_2S-CH_4(a, b) and CO_2-SO_2-N_2(c, d) ternary mixtures systems at 298 K and low pressure area

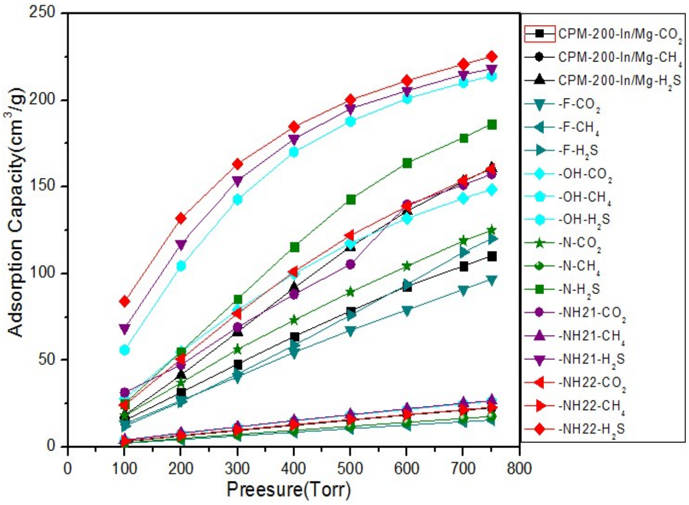
Fig. S6


273K,1bar
CO$_2$ uptake(cm^3/g)
CPM-200-In/Mg
-F
NbO-Pb-1
NJU-Bai21
CPM-200-Fe/Mg
Cu-TPBTM
-NH$_2$(site1)
-OH
-N
Cu-TDPAT
MOF-74-Mg
-NH$_2$(site2)

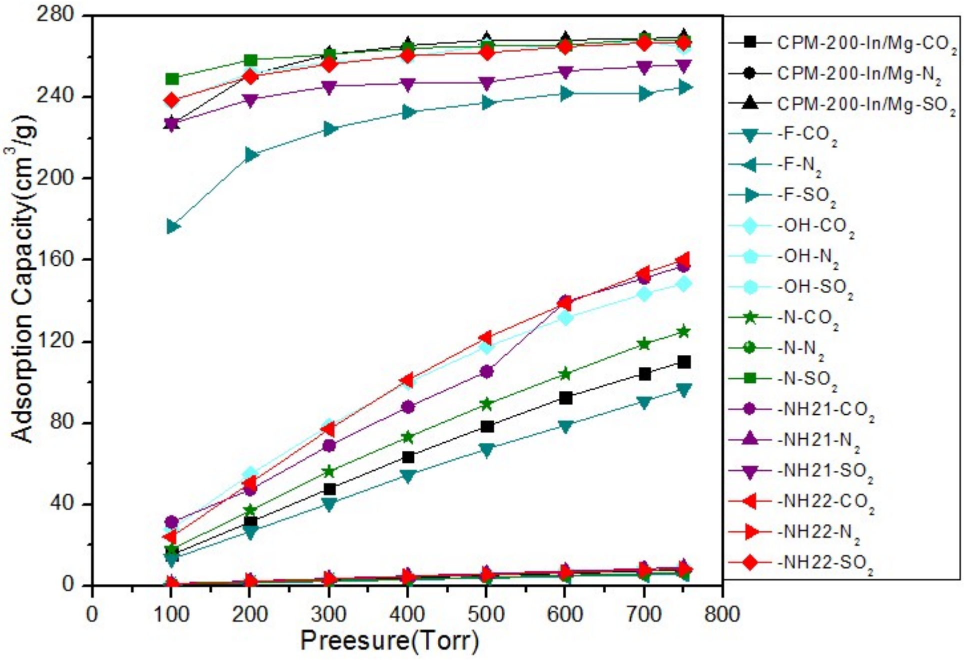
(a)


HCHO uptake(g/g)
298K,1bar
active carbon
438-MOF
CPM-200-In-Mg
-F
-NH$_2$(site1)
-OH
-N
-NH$_2$(site2)

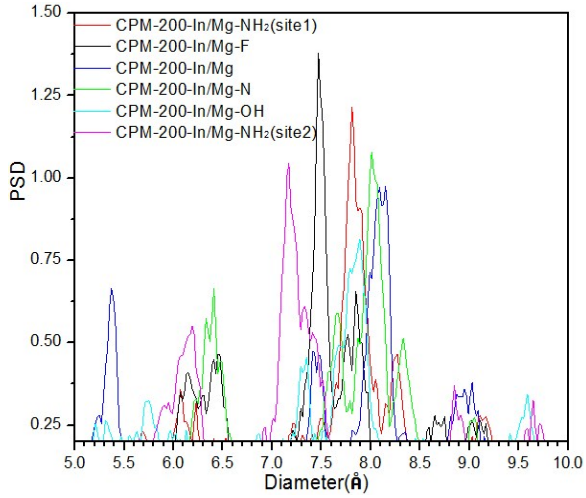
(b)


Adsorption Capacity(cm^3/g)
Preesure(Torr)
CPM-200-In/Mg-CO$_2$
CPM-200-In/Mg-CH$_4$
CPM-200-In/Mg-H$_2$S
-F-CO$_2$
-F-CH$_4$
-F-H$_2$S
-OH-CO$_2$
-OH-CH$_4$
-OH-H$_2$S
-N-CO$_2$
-N-CH$_4$
-N-H$_2$S
-NH21-CO$_2$
-NH21-CH$_4$
-NH21-H$_2$S
-NH22-CO$_2$
-NH22-CH$_4$
-NH22-H$_2$S

(c)


Adsorption Capacity(cm^3/g)
Preesure(Torr)
CPM-200-In/Mg-CO$_2$
CPM-200-In/Mg-N$_2$
CPM-200-In/Mg-SO$_2$
-F-CO$_2$
-F-N$_2$
-F-SO$_2$
-OH-CO$_2$
-OH-N$_2$
-OH-SO$_2$
-N-CO$_2$
-N-N$_2$
-N-SO$_2$
-NH21-CO$_2$
-NH21-N$_2$
-NH21-SO$_2$
-NH22-CO$_2$
-NH22-N$_2$
-NH22-SO$_2$

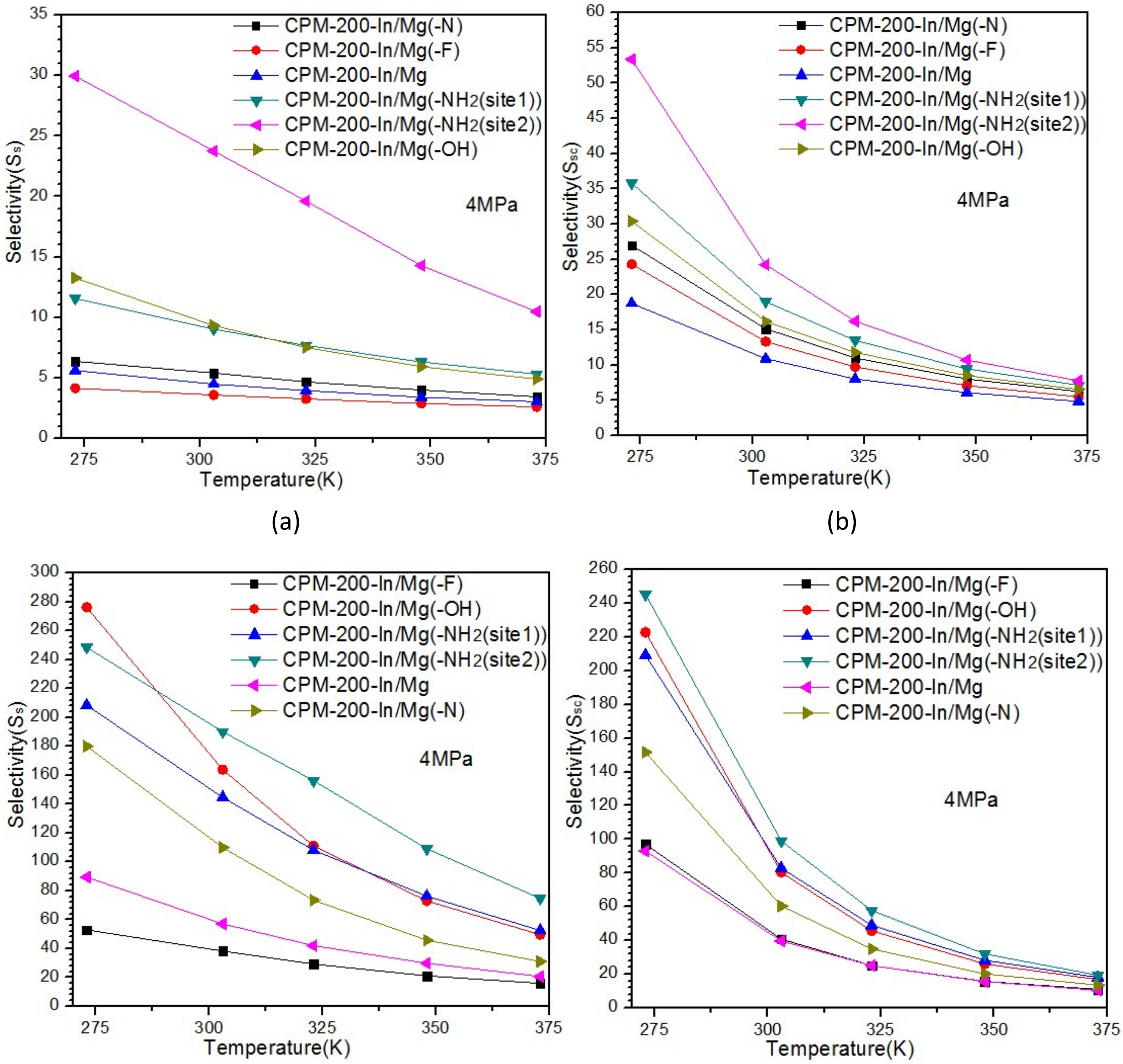
(d)



(e)

Fig. S6 (a) the CO_2 absorption capacity of MOFs at 273 K and 1 bar, (b) the HCHO absorption capacity of MOFs at 298 K and 1bar. (c, d) Single-component adsorption isotherms of CO_2, CH_4, H_2S, N_2, SO_2 in CPM-200-In/Mg and CPM-200-In/Mg-X(-F, -N, -OH, NH_2) at 298 K and low pressure area(within 1 bar). (e)The pore-size distribution of MOFs

Fig. S7



(b) (d)

Fig.S7 The effect of temperature on gas selectivity of materials in CO_2-H_2S-CH_4(a, b) and SO_2-CO_2-N_2 (c, d) ternary mixtures systems at 4 MPa

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