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Designed synthesis of a hydrophobic covalent polymer composite to expel toxic dyes and oil from waste water: A theoretical corroboration

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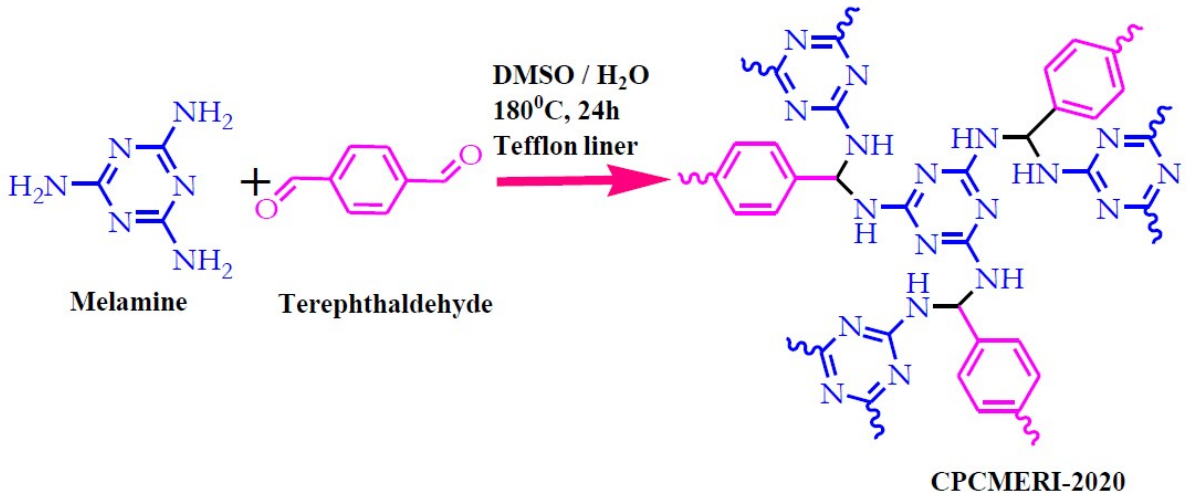

Scheme S1. Synthesis of **CPCMERI-2020**

Table S1. Yield with respect to time and temperature difference

Temperature (°C)	Time (h)	Yield (%)
150	72	78
120	24	47
120	48	64
120	72	78
120	96	78
90	72	64
70	72	52

Table S2. Stoichiometric ratio of starting materials for the preparation of **CPCMERI-2020** with corresponding yield

Stoichiometry (Melamine: Terephthaldehyde)	Reaction condition	Yield (%)
2:3	120°C, 72 hours, Teflon-lined autoclave	65
1:1	120°C, 72 hours, Teflon-lined autoclave	78
3:2	120°C, 72 hours, Teflon-lined autoclave	62

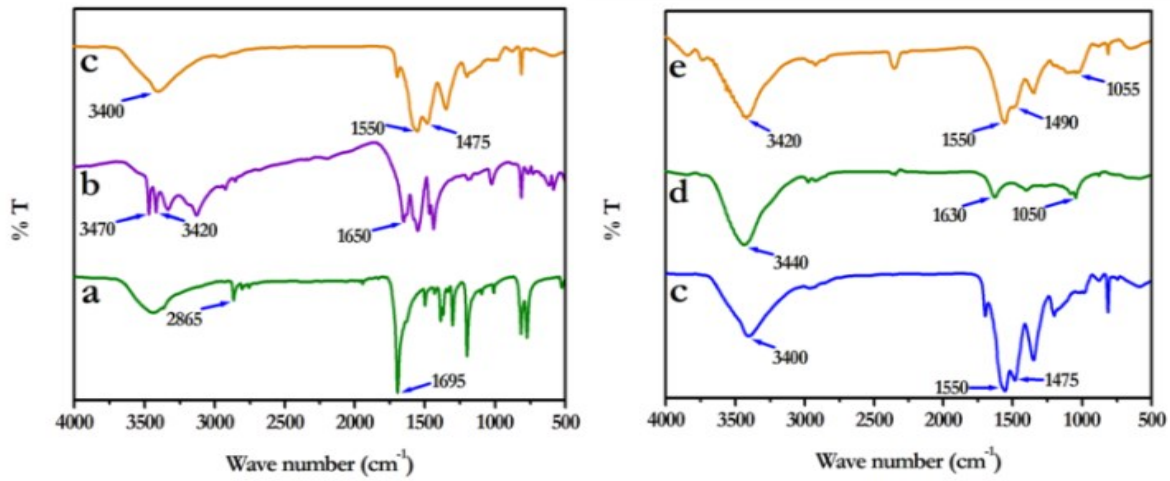

Fig.S1 FT-IR spectra of a) Terephthaldehyde, b) Melamine, c) **CPCMERI-2020**, d) WCS, e) **CPWCS**

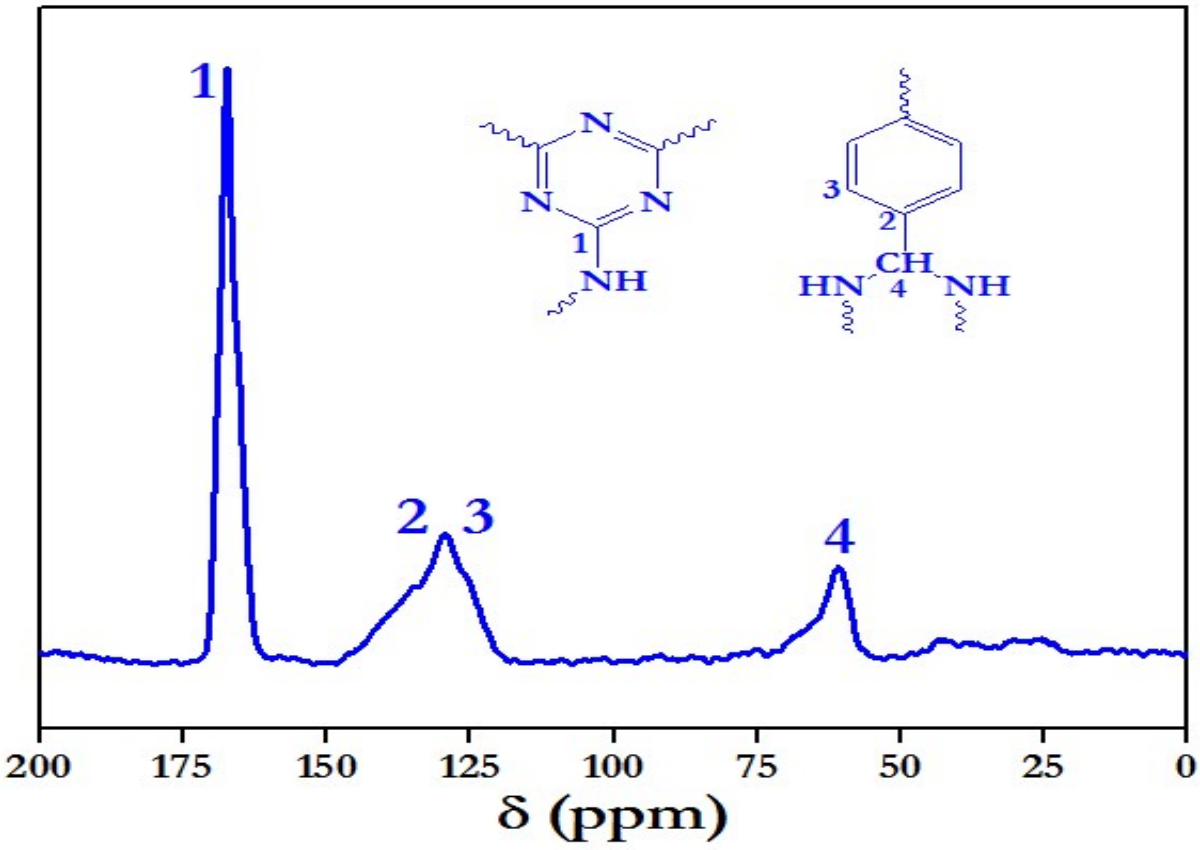

Fig.S2 Solid state ^{13}C NMR spectra of **CPCMERI-2020**

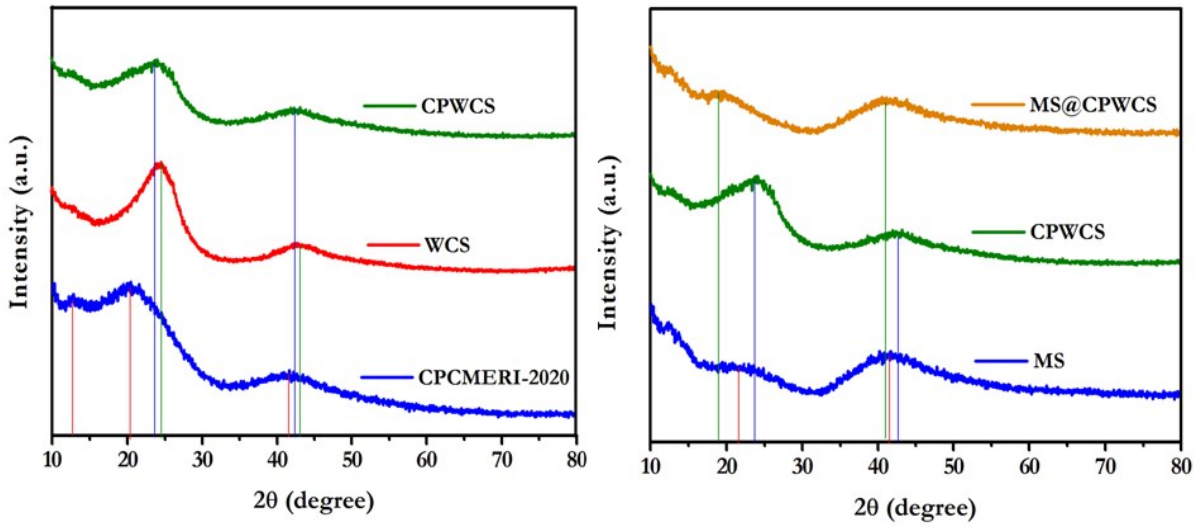

Fig.S3 Comparative PXRD spectra of a) **CPCMERI-2020**, WCS and **CPWCS**, b) MS, **CPWCS**, and **MS@CPWCS**

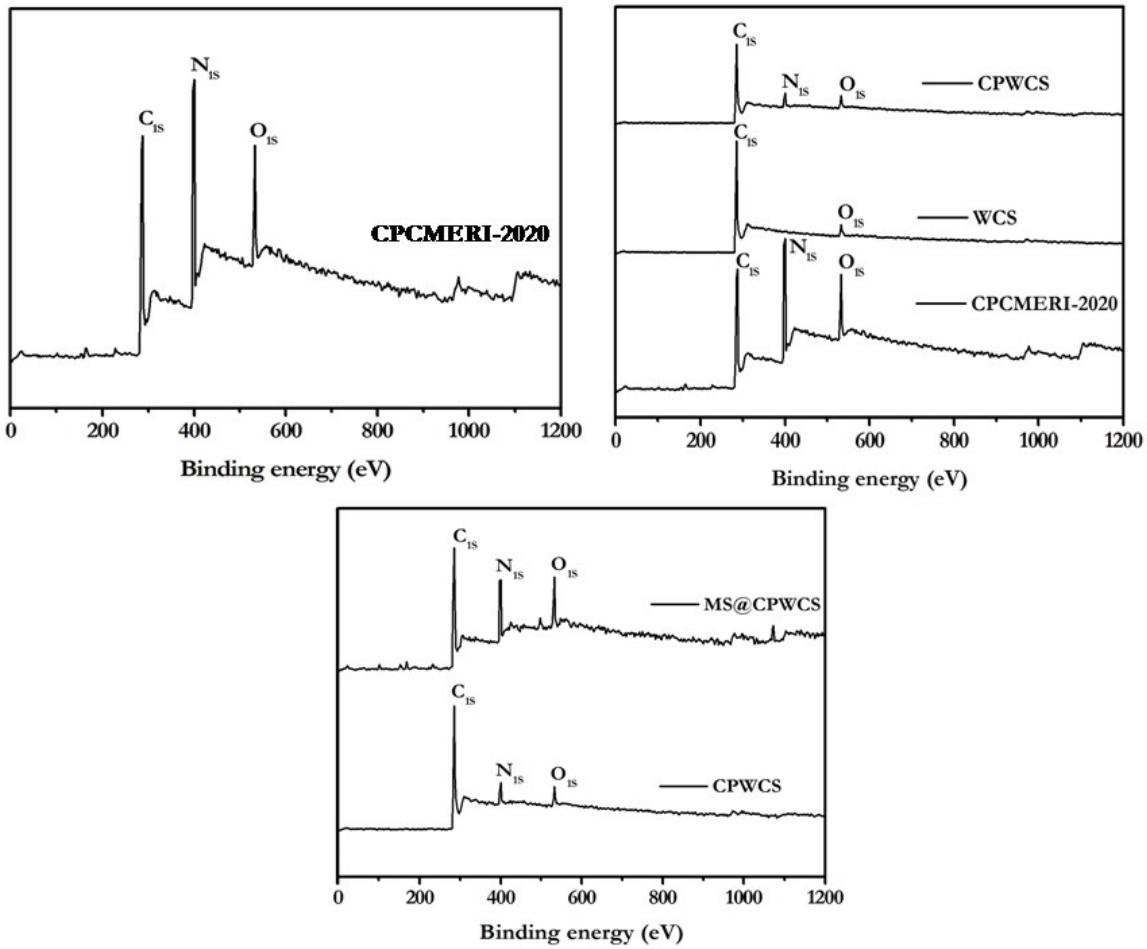

Fig. S4 The C/O molar ratio and elemental contents of the **CPCMERI-2020**, WCS, **CPWCS**, MS, **MS@CPCS**

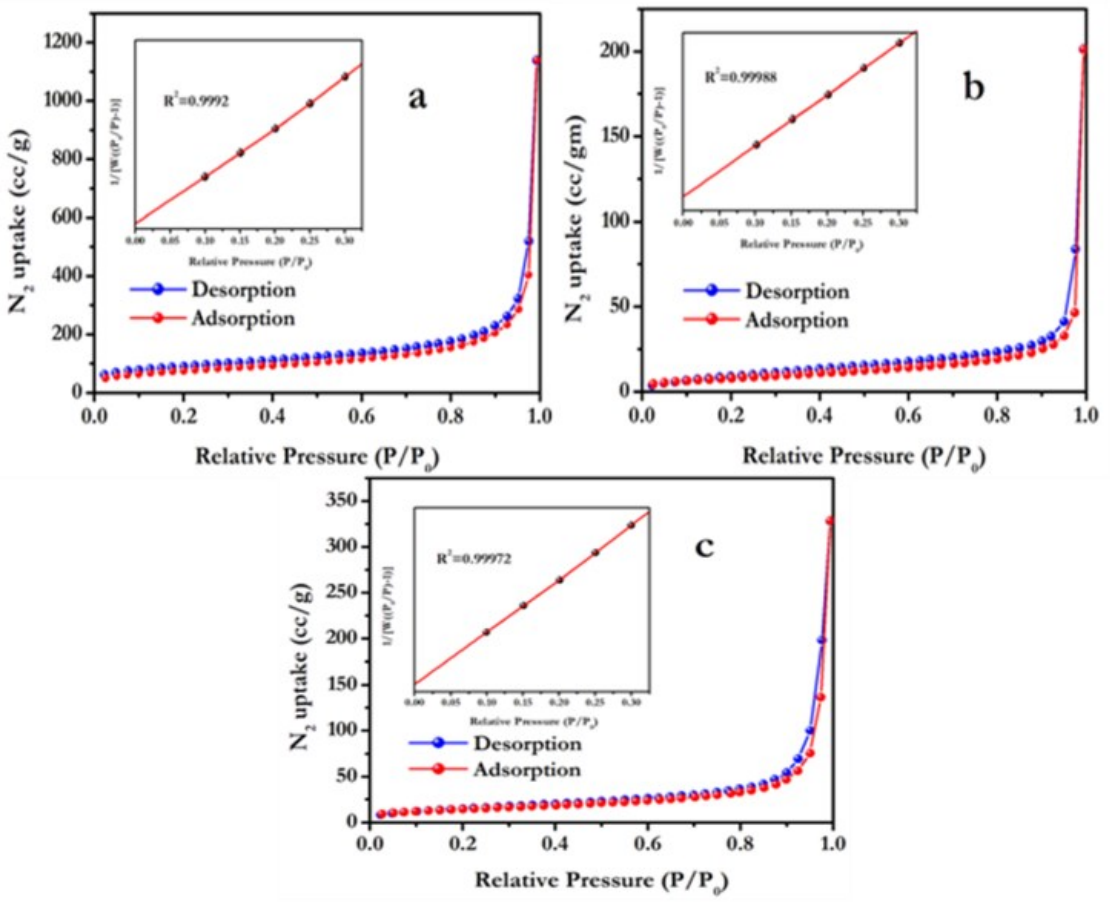

Fig.S5 N_2 adsorption/desorption spectra of a) **CPCMERI-2020**, b) WCS, C) **CPWCS**

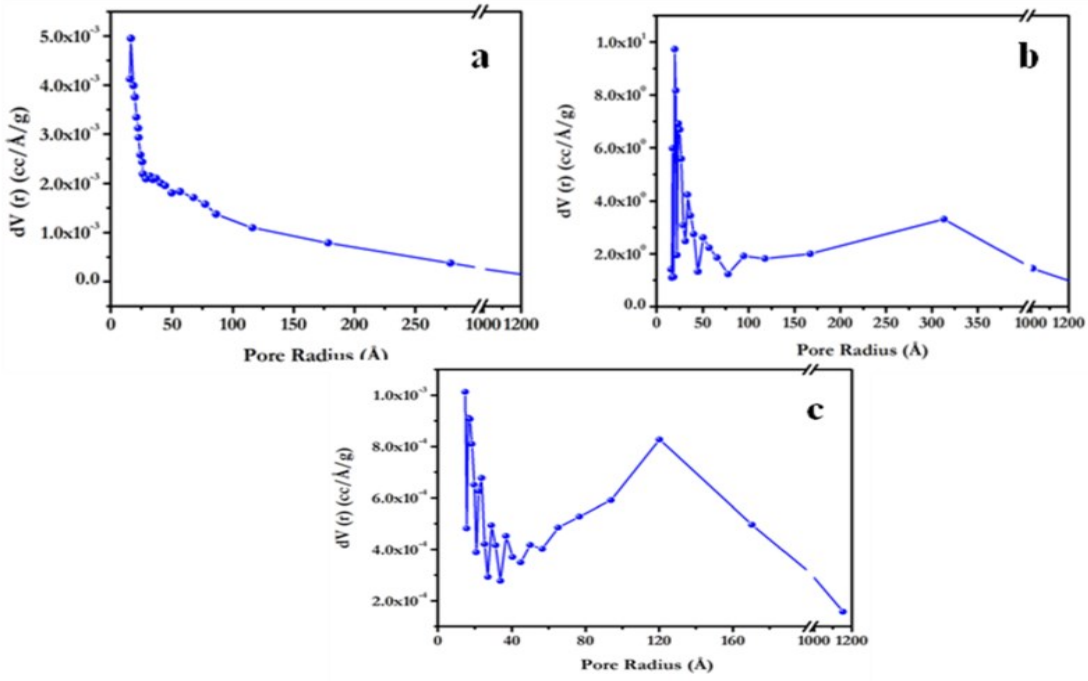

Fig. S6. Pore size of **CPCMERI-2020**, WCS, **CPWCS** (16.576 Å, 15.655 Å, 14.854 Å respectively)

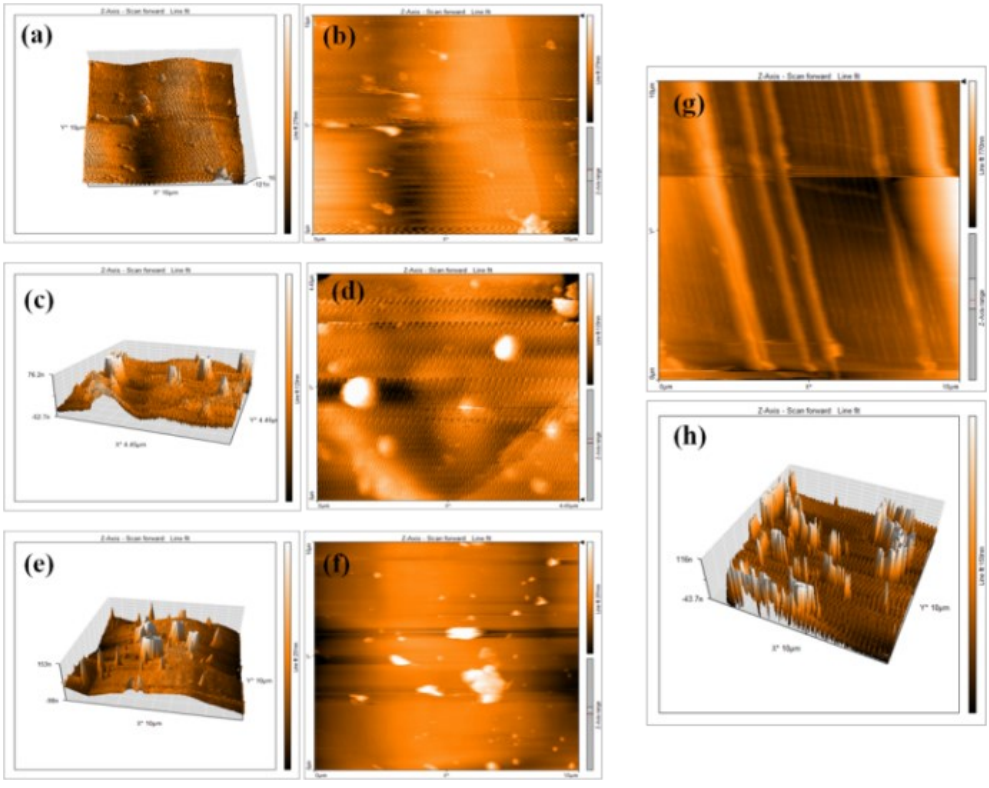

Fig. S7 AFM images of **CPWCS** coated melamine sponge and surface roughness

Contact angle measurement

The contact angle of any liquids on the solid surface can be easily measured by Young's equation:

$$\sigma_{sg} = \sigma_{sl} + \sigma_{lg} \times \cos\Theta$$

$$\sigma_{sg} = \sigma_{sl} + \sigma_{lg} \times \cos\Theta$$

where Θ is the contact angle, σ_{lv} is the surface tautness of the liquid and vapour interface, σ_{sl} is the surface tautness of the solid and liquid interface and σ_{sv} is the surface tautness of the solid vapor interface.

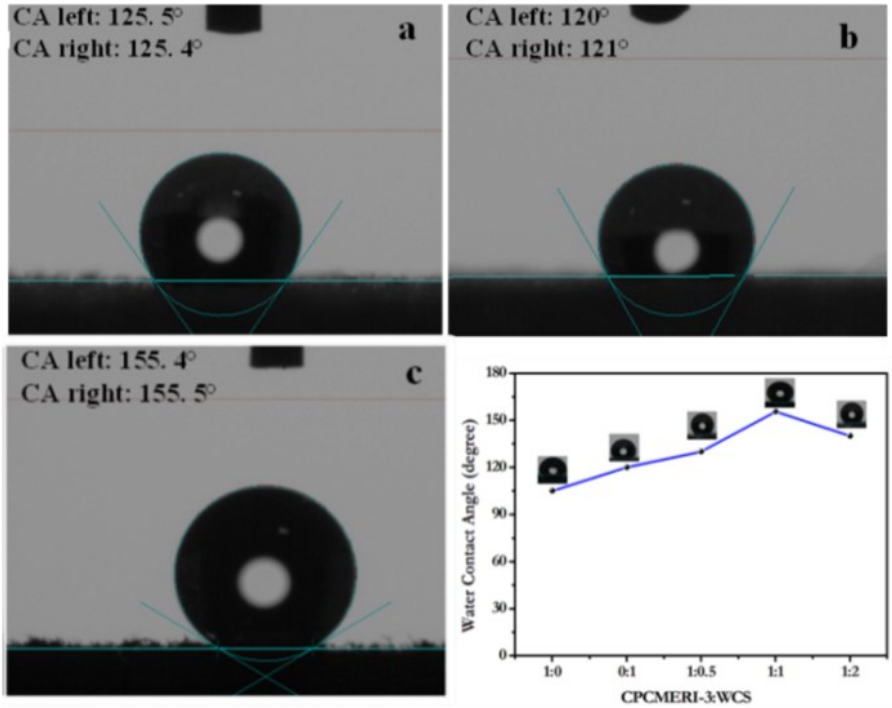

Fig. S8 Contact angle of water droplet (5µL) over (a) **CPCMERI-2020** coated MS, (b) WCS coated MS, (c) **CPWCS** coated MS,(d) Comparison of stoichiometric ratio of **CPCMERI-2020** and WCS with contact angle

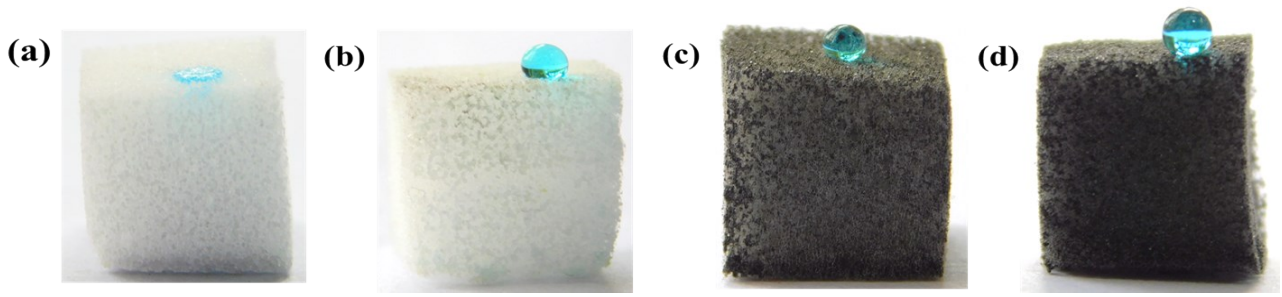

Fig.S9 Physical photos of Contact angle of water droplet (5µL) over (a) MS (b) **CPCMERI-2020** coated MS, (c) WCS coated MS and (d) **CPWCS** coated MS

Dye adsorption capacity measurement

The adsorption ability of the dye was derived from the equation:

$$q_t = \frac{(C_0 - C_t) \times V}{W}$$

where q_t (in mg/g) is the adsorption efficacy of the sorbent materials at any time. C_0 and C_t are respectively dye concentration at initial and dye concentration at time t. V (Litter) is volume of used solution and W (gm) is weight of the covalent polymer (**CPCMERI-2020**).

The adsorption isotherms equations are given bellow:

$$\frac{1}{q_e} = \frac{1}{K_L C_e q_0} + \frac{1}{q_0}$$

$$\ln q_e = \ln K_F + \frac{1}{n} \ln C_e$$

where q_e (mg/g) and C_e(mg/L) are equilibrium adsorption capacity and equilibrium concentration respectively. Here, q_0 is the maximum adsorptivity and K_L (L/mg) is equilibrium adsorption constant.

Dye removal efficiency calculation

In this work, the removal of dye was carried out by stirring the 50 mg adsorbent materials with 50 ml 10^{-5} M ethanol solution of dyes at room temperature and neutral pH followed by simple filtration. In all cases (of various dyes) constant time and equal concentration was maintained. The removal efficiency of the dye can be measured by the following equation:

$$R = \frac{(C_0 - C_e)}{C_0} \times 100\%$$

Where, R= removal efficiency, C_0 (mg/L) is the initial concentration of dye, C_e (mg/L) is the equilibrium concentration of the dye.

Oil adsorption studies

The sorption experiment of toxic oils and solvents have been performed at room temperature. For every adsorption analysis 1×1×1 cm^3 fresh **MS@CPWCS** was taken by weighing and putting it in a beaker containing a measured volume of 5 mL of toxic oil or solvent. After the sorption process reached saturation *i.e.*, after completion of the soaking process, the composite was removed from the solvent and the remaining solvent was measured, from which we can easily calculate the amount of guest adsorbed by the polymer.

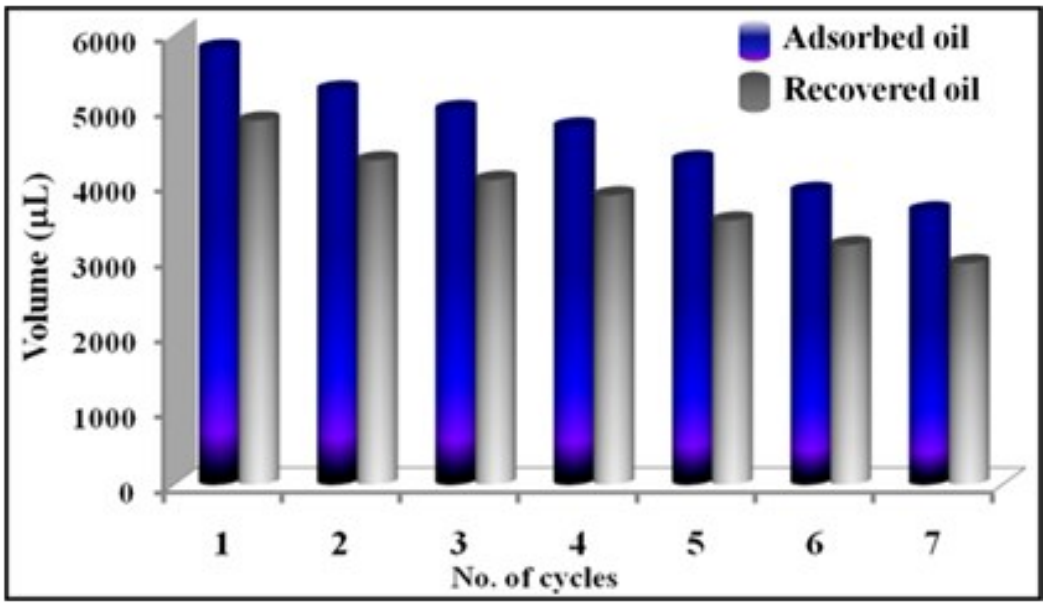

Fig.S10 Recyclability of **MS@CPWCS** towards oil contaminant

Table S3. Cartesian coordinates of **CPCMERI-2020**

ATOM	CARTESIAN COORDINATES		
1 n	-4.57919410218454	5.52803465548442	-0.60821247055987
2 n	-1.70875391750285	2.06750631526190	-0.28252129186456
3 c	-2.67033258586642	4.08591020720618	-1.46044619602582
4 c	-5.55718659761692	4.77795811620005	1.60653712205722
5 n	-4.77833457071537	2.77069795497204	2.94809720325183
6 c	-2.85368717494758	1.48044364640620	1.90603419858408
7 n	-1.65563426949097	4.77323732398177	-3.72967701694893
8 c	0.44159450267541	3.51155587821299	-4.93846950676611
9 n	2.83333944719107	4.46821271753226	-3.91590386497819
10 n	-2.01564206435704	-0.56798241435477	3.20711799033527
11 c	0.00104108675399	-2.23787177919108	2.37466034633866
12 n	-0.65259392488044	-4.86040493284824	2.88080874237427
13 n	-7.52997671761657	6.11183270654707	2.59558632283792
14 c	-8.40560020165404	8.50703262861688	1.63094550480269
15 n	-7.23143120073499	10.66669213308368	2.91095032892584
16 c	0.75113547533976	6.27249310561618	-11.64081626083969
17 c	-0.35570671599910	4.33138895452409	-13.05829024749358
18 c	-1.16422211160786	2.12082365550456	-11.84891202813440
19 c	1.04783772233273	6.00416076193806	-9.02619113033217
20 c	0.23182245345282	3.79795201761881	-7.80118608699422
21 c	-0.87188420669377	1.85956053141650	-9.23382836889410
22 n	6.98772896119706	4.22589640428449	-2.60837638701823
23 n	9.26697648982665	0.41304558046260	-3.27588569730132
24 c	9.03705751251765	2.80169713696961	-2.45745872725561
25 c	4.96656522282551	3.09826710071474	-3.70898569903065
26 n	4.98543846105391	0.70527066619298	-4.60424434145238
27 c	7.15963411986769	-0.50953866521467	-4.32426390272948

28	c	4.77343891316504	-2.36241323077822	2.23855628146254
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30	c	7.38092883090505	-0.78790787163896	5.65940579642159
31	c	2.57616164223755	-1.66703177145490	3.55338281965718
32	c	2.80931701762670	-0.52311775215331	5.93092541190040
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42	c	-6.34696791393381	13.57208649712126	8.76197220582804
43	c	-8.70005942430920	10.09187600271494	9.33448096841337
44	n	-8.64382536983649	9.49092003626872	6.90066662564290
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46	c	-15.44832017782530	6.69766697847567	1.43840814847751
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48	c	-11.29945507417017	8.68571001481324	1.57843636764391
49	c	-16.60378036399071	9.06204318032835	1.18847055025104
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51	c	-12.47429144588607	11.05173826287075	1.31800521434816
52	h	-2.40642435295059	6.32939564207546	-4.56330213218746
53	h	0.35947652034323	1.49732561911581	-4.45165936588544
54	h	2.88160955966158	6.25771867532732	-3.22223407679050
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57	h	-0.08925474229715	-5.65105016545938	4.53756714666449
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63	h	-2.01859367726694	0.58929490934911	-12.94573485756317
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81 h	4.60910613054122	-3.24820599829642	0.37563522560139

Table S4. Cartesian coordinates of **CPCMERI-2020+RhB**

ATOM	CARTESIAN COORDINATES		
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5 n	-5.05914432661688	3.51783539159622	2.39779183049043
6 c	-3.17359885530732	2.00458295532793	1.62989699230538
7 n	-1.25601582776793	4.71374833675340	-4.11756230676785
8 c	0.85009424174506	3.22842882554065	-5.00892340934750
9 n	3.19455682168469	4.10305298702382	-3.81222469357776
10 n	-2.60951445223297	0.02501927322500	3.16596795995946
11 c	-0.74841941851348	-1.92077815594993	2.61536839186123
12 n	-1.75745815598379	-4.41134719566255	3.19181327323085
13 n	-7.54027784671798	6.96928568431374	1.52491725325677
14 c	-8.02506535500514	9.40736999257023	0.41373452123918
15 n	-6.50922390923658	11.43111662278228	1.56154388828475
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17 c	0.93675777484928	3.47063358582778	-13.20628044893471
18 c	-0.18223639074674	1.43614076696128	-11.93619348646808
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21 c	-0.17500480020683	1.35984599227937	-9.29305554432546
22 n	7.16548931055882	3.69238540546366	-2.05406115152655
23 n	9.23894536818462	-0.28771106006560	-2.25218446008420
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25 c	5.19630093393334	2.62172570037945	-3.29792809419619
26 n	5.14574766117756	0.17818125218669	-4.04453391899227
27 c	7.19279932243646	-1.14597735001499	-3.46390286701183
28 c	3.98974305565719	-2.48469856734668	2.88924681895909
29 c	6.31210117093991	-2.24761285668880	4.12759222510088
30 c	6.42948452927239	-1.10205888597845	6.51138426788799
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34 n	-6.17677514375102	-8.53685687745951	-1.47461481978514
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44 n	-8.00359371485952	10.71088436352955	5.63270143308321
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46 c	-15.25770834060336	8.71433304598555	0.25034961802505
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53	h	0.57270649618893	1.26692772625026	-4.39377944433936
54	h	3.28808891040603	5.92487668381368	-3.21410749400455
55	h	-3.72899194619813	-0.17278727255239	4.71108389293451
56	h	-0.41364964100650	-1.83140854028278	0.57129624740778
57	h	-1.55544459216942	-5.09897537964851	4.97316196058634
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68	h	8.03624425236230	-2.93650089788966	3.21679296375021
69	h	8.24516182884693	-0.91054559378220	7.48397827091491
70	h	0.18302669168339	0.33700968342679	7.26256453045363
71	h	4.29325560380531	0.71521110834794	9.49438092088132
72	h	-5.45749808026112	-5.70595288978501	-4.11096690740195
73	h	-6.51753128392056	-10.97457546627929	1.59490467838566
74	h	-3.74320931431614	15.93980001363361	7.90594773570848
75	h	-9.09469853416661	10.40340185387385	9.37121780141394
76	h	-16.66019104951936	7.19546837008104	0.33496740054822
77	h	-12.10686733733552	6.15213133473034	0.66145334784624
78	h	-18.04814779067154	11.68353077467935	-0.18867699929057
79	h	-14.79916507535209	15.11415353553531	-0.38337433836218
80	h	-10.24589641352257	14.06777247108616	-0.03720078880221
81	h	3.90416215215840	-3.38010128738803	1.02557769866876
82	o	-17.12590227590895	-10.00816948097581	-1.42577269862720
83	o	-17.07557841342654	-5.84549959935962	-0.69085833597777
84	c	-9.18884243360866	3.04180990574320	-7.30605109333256
85	c	-11.34178999962686	4.91294548070738	-7.83997567600009
86	c	-9.88976746180525	-1.06555756862732	-9.44421458843827
87	c	-7.36205400685735	-2.40857592130315	-9.92227300616950
88	c	-11.71285189838506	4.71760546842023	11.29127459109766
89	c	-10.24603744440116	2.63160779783577	12.63750832363451
90	c	-15.77088059463656	5.91129565783840	9.48293834340367
91	c	-18.45466978500810	4.95996167578948	9.09636078856690
92	h	-19.88328031164605	6.38699380851129	8.51102637437653
93	h	-18.85977415039875	3.40695266684151	10.69192887249627
94	h	-18.75202227968929	3.42241330855478	7.71027850022855
95	h	-15.77782654931962	7.33214184564594	11.00407460339525
96	h	-15.21958077358678	6.91547574987329	7.72155821496302
97	h	-10.48582959720733	5.60074973664782	9.82534411377494
98	h	-12.17944930202864	6.21807766818748	12.66580436944639
99	h	-9.66647638563825	1.12499713145910	11.31763952252066
100	h	-11.40653808963861	1.76772109646197	14.14317637353697

101	h	-8.52355052617814	3.42969602232981	13.50625877956558
102	h	-18.46838321707046	-9.38947921995947	-2.53435125692688
103	h	-10.59603229385605	6.85819106423136	-8.00758676224220
104	h	-12.31454946624523	4.44023532578875	-9.62737747595581
105	h	-12.76131797705725	4.89386929710402	-6.31011942471990
106	h	-8.18230052741975	3.58848119990468	-5.56347663431088
107	h	-7.77285198450551	3.18041941928411	-8.83383094134718
108	h	-11.44268106502489	-2.45807018492184	-9.43885014260883
109	h	-10.29018102320155	0.21812124492585	-11.04165770158811
110	h	-6.91270322395746	-3.74654917856329	-8.38458153811595
111	h	-5.79898728970057	-1.02903073989537	-10.04744977121912
112	h	-7.42751039636723	-3.47437988471129	-11.71863111250657
113	h	-19.73660556286575	5.04192182534221	10.95026655803537
114	c	-12.97512131841092	2.48580050698438	5.80349485581365
115	c	-12.72543375370537	0.61158247166807	3.98134684069359
116	o	-11.97075588516121	1.40961613315622	1.63379514500179
117	c	-11.79634108495602	-0.27192094851744	-0.34908373254193
118	c	-11.06083793172252	0.81332553984598	-2.63201349951548
119	c	-10.70324376759588	-0.66738436844994	-4.83367063416725
120	c	-11.12818908064375	-3.28825718091854	-4.54461456282850
121	c	-11.90094955269389	-4.31611815326461	-2.23437375491681
122	c	-12.28986548792088	-2.88084648355496	-0.01865576330461
123	c	-12.91913694199908	-3.85940105201899	2.50062395918770
124	c	-13.22725731451578	-1.99687641041537	4.47296878384368
125	c	-14.19170236227497	-2.48299787493441	6.94334145023079
126	c	-14.47517999078799	-0.60285600253791	8.77852229690659
127	c	-13.84653366458918	1.91219907016944	8.26196858917655
128	n	-9.98497733222594	0.41327774027701	-7.12788698665930
129	n	-14.11030112741631	3.83581620277464	10.18565196944581
130	h	-12.46401597710114	4.41927107494070	5.28228427165927
131	h	-10.75545595512464	2.84967626384846	-2.63156685808701
132	h	-10.83380150922943	-4.58411333335389	-6.12178356090607
133	h	-12.10717044415167	-6.36454975766862	-2.13891188337303
134	h	-14.76902218200095	-4.40709929730355	7.41809555466595
135	h	-15.21084772662793	-1.09039593001204	10.65037634029344
136	c	-12.97727395644170	-6.53591397724618	3.09460321089310
137	c	-14.20018196806059	-8.50385776719463	1.63147210022990
138	c	-13.72859995903155	-11.09380284413061	2.20227327743777
139	c	-11.57451745884678	-7.40139241452775	5.24268365434158
140	c	-11.19732524518706	-9.92686570426850	5.79639021926964
141	c	-12.25697251962107	-11.82708880356069	4.23165456892550
142	c	-16.18349045118937	-7.92261663160727	-0.20555024729700
143	h	-14.60999207453026	-12.53268184526094	1.01348950696494
144	h	-10.61478752014841	-5.98303611105562	6.39791419449566
145	h	-10.00007090383220	-10.45359722932186	7.40239585324362
146	h	-11.92526381498918	-13.83073098148034	4.62646835996293

Table S5. Cartesian coordinates of **CPCMERI-2020+MG**

1	n	-4.00796378432282	8.83242892595363	-1.05522871913240
2	n	-1.87702650056275	4.90216304942816	-0.48134324843270
3	c	-2.38401021651410	7.01711822937447	-1.76844147628707
4	c	-5.19362747224922	8.37886424681624	1.13705292044931

5	n	-4.85964653329535	6.32934396916500	2.58753047966496
6	c	-3.19494854591526	4.64438382086416	1.67410720970355
7	n	-1.16207098008599	7.41189181873761	-4.01009929035380
8	c	0.84770405084822	5.84822354155056	-4.98343936614340
9	n	3.25304895415154	6.55502618101793	-3.78746276230609
10	n	-2.81881476068078	2.53018071290011	3.08401168976090
11	c	-0.95093957587788	0.58846280633464	2.53936845619140
12	n	-1.85667364441235	-1.86002263223043	3.39927026220582
13	n	-6.90164065481591	10.11661885998517	1.99677081316318
14	c	-7.13671960811486	12.64572019497168	1.00833580052161
15	n	-5.52682668282886	14.46587451249892	2.34554123780631
16	c	1.82682075896462	8.42990705301800	-11.68646688087860
17	c	1.03185612847668	6.38281143427814	-13.16503204294010
18	c	0.20622749532645	4.16088460098910	-11.99188197122785
19	c	1.79319826560589	8.25323759641193	-9.04908213852334
20	c	0.95018347621270	6.03570912056283	-7.85916976128248
21	c	0.16716670247262	3.99198879136680	-9.35157901453986
22	n	7.28964025326788	5.91591585442667	-2.26493635983579
23	n	9.18180759897048	1.86884204793908	-2.73285014806645
24	c	9.16561621296461	4.28934644417936	-1.97721860177946
25	c	5.21607248397847	4.97708957440481	-3.44426445447496
26	n	5.02609071571583	2.57231252120037	-4.28853233999224
27	c	7.04313526361827	1.14540050448323	-3.87135385838105
28	c	3.80595165478346	0.08563090565361	2.54683166155542
29	c	6.19787200705638	0.43298327825881	3.61443699339530
30	c	6.45570766583401	1.78889708363839	5.87394408205005
31	c	1.64518735321996	1.09172097095182	3.71182713512966
32	c	1.91879895952339	2.45634915302610	5.96578981105082
33	c	4.31130944761682	2.79799109083774	7.04611153840386
34	n	-5.23068447798518	-7.25784757055001	-0.82660812286680
35	n	-3.36492067146899	-3.18261571826644	-0.52950357176625
36	c	-4.46289962262783	-5.05204856155701	-1.79048701917515
37	c	-4.78031300286474	-7.49794211416273	1.65511507793515
38	n	-3.68156773951234	-5.80112607326509	3.12692560070292
39	c	-2.99631507298421	-3.63268730449072	1.95248139912500
40	n	-5.70880036934960	15.88482225770621	9.84695339320825
41	n	-3.94911853067144	16.63840432268020	5.78456073584999
42	c	-4.10564218151990	17.02696819936403	8.25052698644962
43	c	-7.22900407365746	14.20202597955013	8.73479287669623
44	n	-7.27012554560307	13.62683872898590	6.29412265773856
45	c	-5.59535489763474	14.91334078055990	4.85406729123324
46	c	-14.37708792265708	12.55306546775999	0.39466484483359
47	c	-11.87072378102198	11.74985550542182	0.67639689843758
48	c	-9.89841827108051	13.51363701075963	0.84646897681063
49	c	-14.94621406436678	15.13183756684602	0.26818402704032
50	c	-12.98615730565974	16.90300357095724	0.42161572595847
51	c	-10.48438710044817	16.09810180141302	0.70718911168691
52	c	-11.89724293425483	-11.39112631541434	4.97789226243081
53	c	-11.36246164323680	-10.20097194193564	9.53650685206285
54	c	-9.28738337843669	0.66432921911860	0.50678599853587
55	c	-11.35941171810674	1.83700279999576	1.73633685972329
56	c	-12.25733483372290	1.02510781277090	4.22666303169684
57	c	-13.13577081938503	2.94701376268911	6.02556746094327

58	c	-15.15462914428548	2.49247815608463	7.73324830107836
59	c	-15.98085639232020	4.34739354637672	9.41836806519422
60	c	-14.81983065716812	6.72913802328073	9.47688432670342
61	c	-12.81218688141551	7.22050220883234	7.81718721712078
62	c	-11.98762198100761	5.37221232873499	6.12695283349810
63	c	-12.46511404978263	3.88320768129635	0.41309319901540
64	c	-11.57430801822625	4.70942825954273	-1.92007567453346
65	c	-9.44606700855468	3.57073012934135	-3.09651438162551
66	c	-8.35548789838740	1.48632824029843	-1.80238196226418
67	n	-8.46818792128286	4.49447508563332	-5.34669480455306
68	c	-6.98394383388602	2.92191305042424	-7.03655113103107
69	c	-9.58624045777476	6.70877179453851	-6.51109577405001
70	c	-12.43536555766866	-3.60595544312269	3.11287652674424
71	c	-12.20240760761805	-1.64207186186191	4.92912775636637
72	c	-11.86185655935332	-2.46371944408383	7.46268569276225
73	c	-12.32446555637973	-6.15161749633383	3.74781369498011
74	c	-11.96580863219707	-6.94756823191049	6.28997110008945
75	c	-11.74132525850561	-5.00066614704944	8.13007265735284
76	n	-11.84393135721020	-9.46853366114746	6.93534061872697
77	h	-1.57312774838670	9.05393551661208	-4.91262382596599
78	h	0.47463277641900	3.88331251639407	-4.43797947812040
79	h	3.46327098357231	8.35315264867469	-3.14796561717791
80	h	-3.82625472643175	2.41637469777475	4.71199172211352
81	h	-0.76037036581817	0.49903745728491	0.47698218221437
82	h	-1.58677151089312	-2.33603674101935	5.24085008701845
83	h	-7.57453831852599	9.82191888493262	3.77100435124639
84	h	-6.35744412357437	12.57203514908353	-0.91483807982157
85	h	-4.15921140604809	15.38147218367136	1.36048634605007
86	h	2.48590333876054	10.16963269119459	-12.59079716264666
87	h	1.06682907693848	6.51734489014811	-15.22891243588737
88	h	-0.40283059918325	2.54726690021035	-13.13378044550204
89	h	2.44943669259051	9.85573162697570	-7.91535485040419
90	h	-0.46538768182394	2.24440775871661	-8.44278622228785
91	h	10.87556677872798	4.98962881339297	-1.02984391622759
92	h	6.94679212498187	-0.82110705492015	-4.53158967545721
93	h	7.86688386963005	-0.33707129243125	2.66671726802904
94	h	8.32676682843974	2.06677292842340	6.71128171633497
95	h	0.25871631457495	3.27887528266978	6.88318887847718
96	h	4.49654382890867	3.86605315850741	8.80813630467463
97	h	-4.77271601377930	-4.75177271175129	-3.82116726913534
98	h	-5.37455667677067	-9.27371258945138	2.55270243573156
99	h	-2.79667866755374	18.41732926127744	9.06548627072320
100	h	-8.57016255997299	13.18974928463699	9.95398275803196
101	h	-15.89364528389922	11.15043771359843	0.27706257860210
102	h	-11.44374482998929	9.73078795404260	0.76359776585082
103	h	-16.90524613959183	15.75967625914302	0.05080824284972
104	h	-13.40425505098546	18.92674725239270	0.32185530875594
105	h	-8.97121596121226	17.50054875932269	0.82739736532706
106	h	3.61266226603829	-0.97307913873018	0.77927072678420
107	h	-13.66425559834338	-11.31456539033816	3.86122727718415
108	h	-11.78503940862915	-13.27031401561727	5.85791336858474
109	h	-10.29333775561141	-11.20487706310204	3.64014859977417
110	h	-9.50758231968744	-9.51110148777831	10.22667135428499

111	h	-11.37005033307077	-12.27438974618513	9.67765829422161
112	h	-12.83352955410552	-9.46787053147799	10.83012300232376
113	h	-5.88681510618017	1.50473149225806	-5.99110564094806
114	h	-5.62475474328184	4.10762666428353	-8.08312703858984
115	h	-8.18082082179418	1.91269682299936	-8.43849875443840
116	h	-8.31273611861283	7.40013348515724	-8.00692797280559
117	h	-9.81501073876312	8.24249346518318	-5.11873010352017
118	h	-11.45930995554244	6.32712614278901	-7.38426441767683
119	h	-8.31450433240904	-0.89453175144130	1.45009993550864
120	h	-16.11488966440502	0.66262780827454	7.69625321214445
121	h	-17.56194304460432	3.93685753285853	10.68966750879219
122	h	-15.47032931664314	8.18127892507454	10.79856846460622
123	h	-11.87029517437178	9.06446305876591	7.84603856148980
124	h	-10.38437506189975	5.76652720050318	4.88298418400692
125	h	-14.11099640293580	4.83694054770663	1.22404950787688
126	h	-12.56709643890951	6.26231636880784	-2.84266658434668
127	h	-6.67711969176857	0.54501803919648	-2.54075862670917
128	h	-12.74578643998773	-3.11029313262088	1.13094950518033
129	h	-11.62459195753793	-1.05542878374548	8.95652967640742
130	h	-12.53311293790258	-7.54229135786594	2.24005770784146
131	h	-11.43497966432815	-5.47324807586375	10.11368489497193

Table S6. Cartesian coordinates of **CPCMERI-2020+MB**

ATOM		CARTESIAN COORDINATES		
1	n	0.00197700668098	7.94127639139070	-4.29905267293529
2	n	2.10060559492540	3.97454083168264	-4.73698082373289
3	c	1.90759649613315	6.46912547120289	-5.10878887280447
4	c	-1.83509218426542	6.70856361166917	-3.06840557631580
5	n	-1.87007603667881	4.21389345315982	-2.60970749751990
6	c	0.15117516578452	2.94436323197874	-3.48385506948605
7	n	3.78018363086200	7.66216357366617	-6.41547448383522
8	c	6.02600439448817	6.44916482420867	-7.38702590733299
9	n	7.94840373559875	6.29346330021985	-5.40255333275156
10	n	0.19193795585649	0.41627279129085	-3.03195038287127
11	c	2.15798957704282	-1.30411889779915	-3.88991246191136
12	n	1.04785347393201	-3.71022690342239	-4.62319228178645
13	n	-3.87523066123719	8.05321151916215	-2.23302150140259
14	c	-3.95099692577215	10.78027549969109	-2.11308475447364
15	n	-2.97621610354757	11.76242060385211	0.28852351836689
16	c	9.43059414638529	11.08129150798003	-11.82956777672158
17	c	8.36171278395443	10.44101059832435	-14.16206308922160
18	c	6.57289537983394	8.49322796340321	-14.29478470910388
19	c	8.71602540712515	9.78120997297678	-9.63740339632931
20	c	6.92242533807678	7.83499893872209	-9.75669520238084
21	c	5.85855908400621	7.20120049336597	-12.10312803859103
22	n	11.25946400711156	4.50748923368565	-3.19480425414961
23	n	13.20952976574671	0.79667326284254	-4.80850561622645
24	c	12.94442317826064	2.66205003281694	-3.11224605119357
25	c	9.68718737868851	4.44445981717462	-5.21657995211816
26	n	9.78099995748361	2.65508997292916	-7.03702378702486
27	c	11.55456624830363	0.91328100208073	-6.71527514975064

28	c	6.61252066324623	-2.63850309832997	-2.80098131903061
29	c	8.54928397474209	-3.16197659835832	-1.08231532196633
30	c	8.13557779323359	-2.85020395730178	1.51439063237232
31	c	4.24542517858933	-1.79088330781926	-1.95266197614746
32	c	3.84760870282051	-1.47469289085496	0.64579043942542
33	c	5.78184682788056	-2.00740712880364	2.37314791254884
34	n	-2.57761220446804	-5.07575529355636	-11.20382754059817
35	n	-0.24254355278102	-2.28077866782118	-8.57620674299181
36	c	-1.45442219944901	-2.86987071852538	-10.69153819749176
37	c	-2.36130715169303	-6.79070052906929	-9.34931104260584
38	n	-1.19076031887883	-6.45835974142598	-7.16312327017534
39	c	-0.15250118965346	-4.14328324384751	-6.83761813722054
40	n	-5.61599596059214	9.85625278768929	7.19340301399328
41	n	-2.68209955589814	12.09259046747890	4.63381127361230
42	c	-3.63251659267182	11.39506102994395	6.83980476738640
43	c	-6.63983467958123	8.99807069529087	5.04908629247507
44	n	-5.86890294395704	9.53297860539009	2.72518017144057
45	c	-3.86814937682535	11.11604231217260	2.58765242741745
46	c	-10.57826181862153	11.47329428959235	-5.01232056254466
47	c	-8.24454216458749	10.44968612474145	-4.29928213033730
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49	c	-11.26777552548996	13.89873009806298	-4.21729442282341
50	c	-9.60164720279106	15.29362972843486	-2.70738172053530
51	c	-7.27253632564759	14.26637409645783	-1.99516424200675
52	c	-10.04658343124722	-1.89777148037366	8.21757076419224
53	c	-9.16202993000761	-1.28248609158906	5.74917556256612
54	n	-10.09874225346936	-2.61147290819598	3.77172597560040
55	c	-9.46571384651980	-2.24288484527573	1.38502108107707
56	c	-10.52288260649591	-3.88853022189484	-0.54034678532064
57	c	-10.10077715076159	-3.74621418351474	-3.09809302537295
58	c	-8.50664389847250	-1.63451679277938	-3.85071139372536
59	c	-7.18684035610971	-0.07512101610572	-2.04631914399247
60	c	-7.67997175303599	-0.34179622206913	0.49821662595490
61	s	-6.11414212998498	1.64462031973742	2.64717023580849
62	c	-7.34910645372619	0.71445307579739	5.58809957691395
63	c	-6.49990403398447	1.98850579910948	7.73213464780530
64	c	-7.41477951888688	1.35753455308034	10.17675949003168
65	c	-9.22922939972340	-0.65266060275388	10.34819573810939
66	n	-6.60430980747382	2.60502635231029	12.27915636211918
67	c	-4.73544609153347	4.61994381590318	12.06688058459167
68	c	-7.54447000297721	1.89965586745502	14.77263206696087
69	n	-8.24237317564154	-1.07708973697343	-6.34292373502167
70	c	-9.47736587488967	-2.55325140598770	-8.31849306229192
71	c	-6.74326082751986	1.06951579924252	-7.21305585736087
72	h	3.59177152983802	9.55971759214466	-6.62739709209794
73	h	5.53967684755655	4.49684795094938	-7.89235142780787
74	h	7.92431459308001	7.60475722775598	-4.00075727001871
75	h	-1.27323772019664	-0.29578580040163	-2.01889666948208
76	h	2.99096643590498	-0.43150133201807	-5.57794302267327
77	h	1.02440397408780	-5.14346606302429	-3.34538418916032
78	h	-5.08022742817021	7.11631032010812	-1.06574568375601
79	h	-2.59722138277528	11.44724388563855	-3.53843304717853
80	h	-1.38894207706445	12.83925518711994	0.26501593832706

81	h	10.83398844017634	12.59635529068314	-11.71099081210002
82	h	8.92644449164995	11.45103416525367	-15.87666307304158
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85	h	4.46208306643030	5.67769428621328	-12.21703926784843
86	h	14.25236097772098	2.65951212982876	-1.49960858768517
87	h	11.67623857893124	-0.57145457882585	-8.16177550393239
88	h	10.39405677485803	-3.79023414858971	-1.77353256925981
89	h	9.65074192180561	-3.25477660405322	2.86332944795546
90	h	2.02348990882153	-0.79022979226520	1.33505875053536
91	h	5.44476539769249	-1.75274703608043	4.39814455231840
92	h	-1.55043629549772	-1.39945341152352	-12.15375840368888
93	h	-3.23937654800685	-8.64376169771383	-9.67185351830185
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101	h	-5.85180240880148	1.38772592831827	-2.63437844785964
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106	h	-6.67668684120529	3.13587631658245	16.19704328350696
107	h	-7.06405159709519	-0.07805323777646	15.24929464687353
108	h	-9.61809501984109	2.11949696980226	14.90281378000513
109	h	-11.43078105130902	-3.42517353297331	8.36429965145408
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112	h	-6.96369533018006	1.25451791756112	-9.27035905806644
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115	h	-10.38374744580030	-4.18621713004500	-7.41020342223759
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117	h	-7.38348871564318	2.84863621447351	-6.32990508496384
118	h	-7.72180814739913	8.55557411017842	-4.93668090978773