Electronic Supplementary Information

Two Facile Aniline-Based Hypercrosslinked Polymer Adsorbents for Highly Efficient Iodine Capture and Removal

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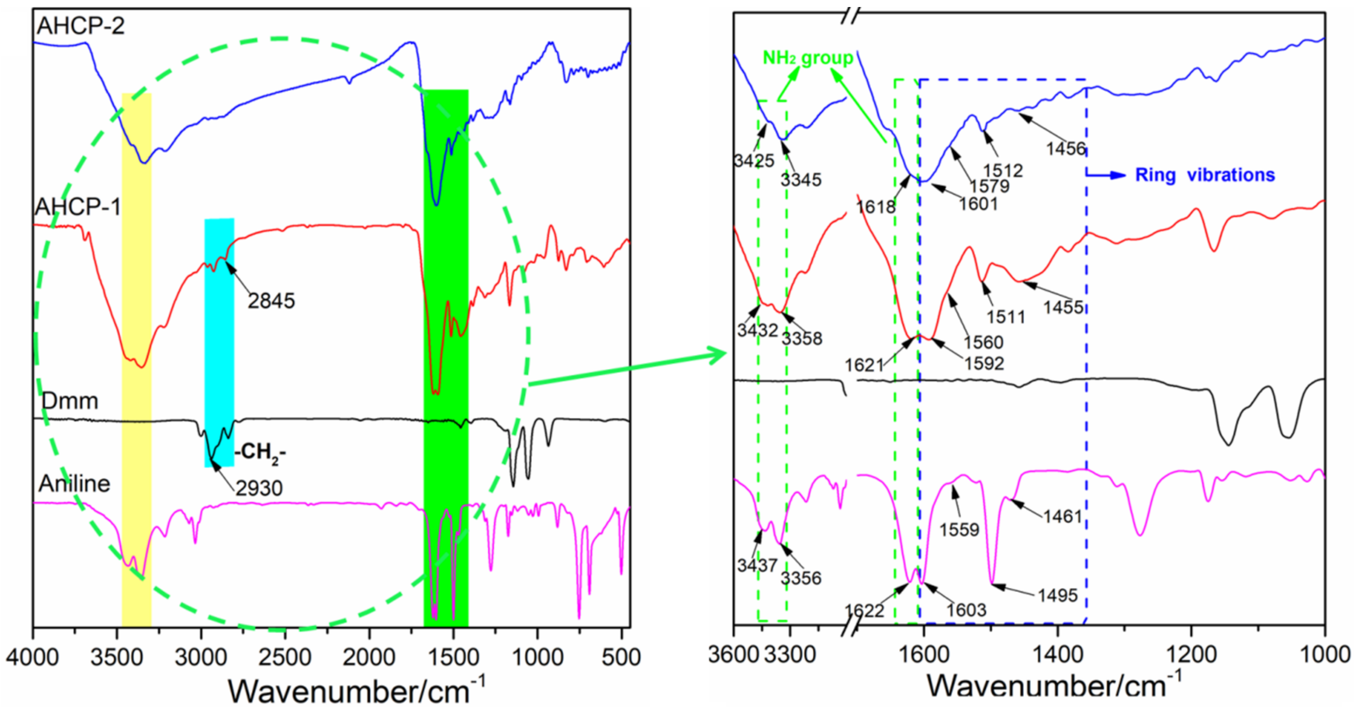

Fig. S1. FT-IR spectra of Aniline(purple), dimethoxymethane (Dmm) (black), AHCP-1(red), and AHCP-2(blue).

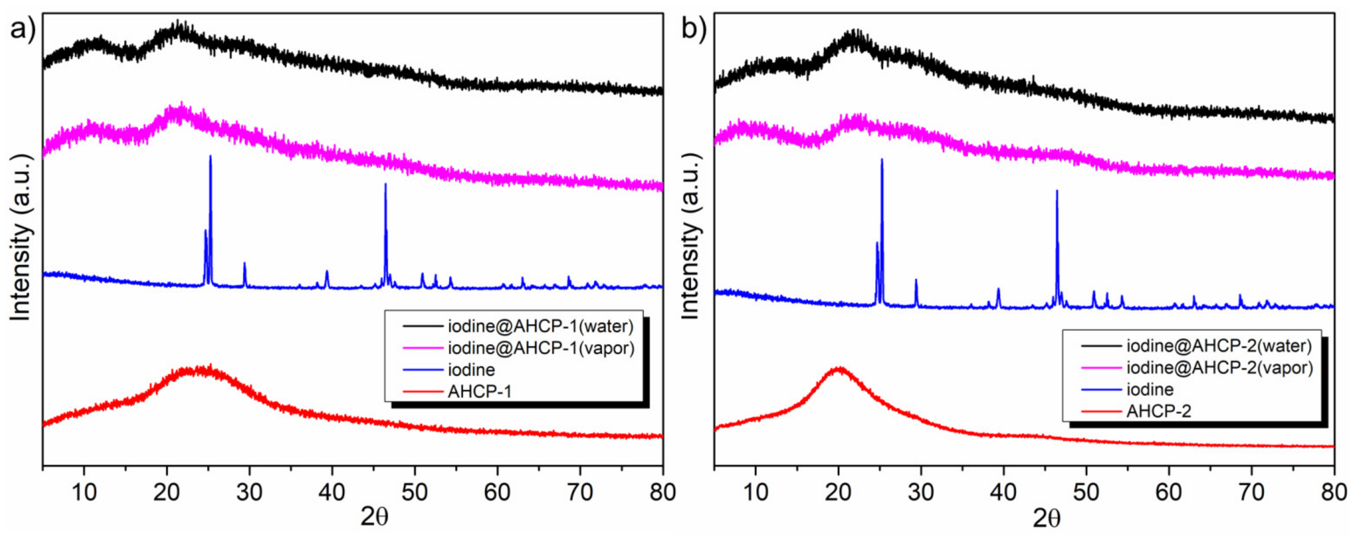

Fig. S2. Comparison of PXRD patterns of (a) AHCP-1 and (b) AHCP-2 before and after iodine adsorption.

Table S1. Iodine adsorption capacity of reported amorphous adsorbents in iodine aqueous solution

No.	Adsorbent	BET(m^2/g)	Iodine adsorption capacity (wt%)	Reference (DOI)
1	**AHCP-1**	**14.4**	**250**	**This work**
2	Fe_3O_4@PPy	30	162.7	10.1016j.jhazmat.2017.10.065
3	**AHCP-2**	**75.2**	**160**	**This work**
4	BC@Dopa-ZIF	1453.3	131	10.1021/acs.cgd.7b01360
5	Activated Bamboo	-	118	10.1016/S0008-6223(00)00230-X
6	Activated Salsola vermiculata plant	-	117.8	10.1016/j.w atres.2014.10.021
7	Activated Coconut shell	-	117	10.1016/S0008-6223(00)00230-X
8	bituminous coal-based granular (GAC-B)	960	101.6	10.1016S0008-6223(99)00180-3
9	Activated Japanese cedar	590	95	10.1016/S0008-6223(00)00230-X
10	activated carbon the granular carbon made of coconut shells (GAC-C)	940	94	10.1016S0008-6223(99)00180-3
11	THPS-C	3125	92.6	10.1002/admi.201900249
12	The activated carbon fabric made from PAN(ACF)	970	88.9	10.1016S0008-6223(99)00180-3
13	Activated Vinylidene film	714	85	10.1016/S0008-6223(00)00230-X
14	Activated Evergreen oak	-	85	10.1016/S0008-6223(00)00230-X
15	Merck activated carbon	-	20	10.1016/j.w atres.2014.10.021
16	n-CF@OCDs	-	19.01	10.1016/j.jhazmat.2019.01.037
17	im-SCMNPs	-	14.1	10.1007/BF03353693
18	n-CF	-	2.81	10.1016/j.jhazmat.2019.01.037
19	PHCP@PES	13.75	18	10.1016/j.jhazmat.2022.128859
20	CTF-DPA	943	66.7	10.1016/j.jece.2022.107805
21	P-TzTz	137	49.09	10.1016/j.micromeso.2020.110161

Table S2. Iodine adsorption capacity of reported amorphous adsorbents in iodine vapor

No.	Adsorbent	BET (m^2/g)	Iodine adsorption capacity (wt%)	Reference (DOI)
1	**AHCP-1**	**14.4**	**536**	**This work**
2	**AHCP-2**	**75.2**	**596**	**This work**
3	TTPPA	512.39	490	10.1039/c7ta08251g
4	TTPB	222	443	10.1039/C7TA00590C
5	CTF-DPA	943	512	10.1016/j.jece.2022.107805
6	HCP	584	460	10.1016/j.seppur. 2018.09.041
7	BPPOC	-	564	10.1021/jacs.2c03959
8	CMP-4	9.5	208	10.1002/ange.202015162
9	PHF-1-Ct	690	405	10.1039/C8CC07529H
10	C-poly-15	96.16	574	10.1039/D1SC05361B
11	PHCP@PES	13.75	77	10.1016/j.jhazmat.2022.128859
12	P-TzTz	137	326	10.1016/j.micromeso.2020.110161
13	CSU-CPOPs-1	1032	494	10.1021/acsami.9b07679
14	FcTz-POP	-	264	10.1016/j.micromeso.2021.110929
15	C-poly-15	96.16	574	10.1039/d1sc05361b
16	PZ-HCP-1:4	209	333	10.1016/j.micromeso.2022.112157
17	ImCMP-1	356.9	236	10.1016/j.micromeso.2022.111871
18	TTDAB	1.643	313	10.1039/c7ta08251g
19	Tm-MTDAB	2.778	304	10.1039/c7ta08251g
20	CalPOF-1	303	477	10.1021/acssuschemeng.8b05203
21	CalPOF-2	154	406	10.1021/acssuschemeng.8b05203
22	CalPOF-3	91	353	10.1021/acssuschemeng.8b05203
23	NDB-H	116.93	443	10.1002/asia.201800698
24	NDB-S	56.45	425	10.1002/asia.201800698
25	ADB-HS	148.2	345	10.1002/asia.201800698
26	ADB-S	41.53	342	10.1002/asia.201800698
27	POP-1	12	357	10.1016/j.jhazmat.2017.05.041
28	POP-2	41	382	10.1016/j.jhazmat.2017.05.041
29	HCMP-1	430	159	10.1021/acs.macromol.6b00901
30	HCMP-2	153	281	10.1021/acs.macromol.6b00901
31	HCMP-3	82	316	10.1021/acs.macromol.6b00901

32	HCMP-4	28	222	10.1021/acs.macromol.6b00901
33	CalP4_Li	445	312	10.1021/acs.chemmater.7b03449
34	TBIM	8.12	943	10.1039/c9ta11982e
35	AzoPPN	400	290	10.1002/chem.201602337
36	Azo-Trip	510.4	238	10.1039/C5PY01671A
37	CMP-E1	2150	215	10.1002/anie.201503362
38	PAF-21	1520	152	10.1002/anie.201503362
39	PAF-23	82	271	10.1002/anie.201503362
40	PAF-24	136	276	10.1002/anie.201503362
41	PAF-25	262	260	10.1002/anie.201503362
42	NAPOP-1	657	206	10.1002/pola.28028
43	NAPOP-2	458	205	10.1002/pola.28028
44	NAPOP-3	702	241	10.1002/pola.28028
45	NAPOP-4	626	265	10.1002/pola.28028
46	CMPN-1	230	97	10.1039/C4TA04235B
47	CMPN-2	339	110	10.1039/C4TA04235B
48	CMPN-3	1368	208	10.1039/C4TA04235B
49	NiP-CMP	2630	202	10.1039/c4cc01783h
50	PAF-1	5600	186	10.1039/C4TA00049H, 10.1002/anie.200904637
51	JUC-Z2	2081	144	10.1039/C4TA00049H, 10.1039C1JM12545A
52	CMOP-1	431	160	10.3390/molecules23071732
53	CMOP-2	406	93	10.3390/molecules23071732
54	NTP	1067	180	10.1021/acsmacrolett.6b00567
55	AK-1	1634	237	10.1016j.jhazmat.2016.09.015
56	AK-2	2751	262	10.1016j.jhazmat.2016.09.015
57	AK-3	2016	253	10.1016j.jhazmat.2016.09.015
58	PAN1	618	133	10.1002app.46106
59	PAN2	542	245	10.1002app.46106
60	PAN3	194	281	10.1002app.46106
61	PAN4	522	237	10.1002app.46106
62	PAN5	439	189	10.1002app.46106
63	Cg-5P	840	8.7	10.1039c1ra00351h
64	Cg-5C	1290	23.6	10.1039c1ra00351h
65	SCMP-1	418	188	10.1021acsami.6b06569

66	SCMP-2	855	220	10.1021acsami.6b06569
67	SCMP-II	119.76	354	10.1039/C6CC05188J
68	BQCMP-1	422	151	10.1002/mame.201600138
69	BQCMP-2	123	161	10.1002/mame.201600138
70	FCMP-600@1	551	108	10.1038/s41598-017-14598-0
71	FCMP-600@2	636	141	10.1038/s41598-017-14598-0
72	FCMP-600@3	629	90	10.1038/s41598-017-14598-0
73	FCMP-600@4	88	111	10.1038/s41598-017-14598-0
74	NCMP1	58	215	10.1021/acsami.7b09553
75	NCMP2	280	186	10.1021/acsami.7b09553
76	NCMP3	485	161	10.1021/acsami.7b09553
77	NOP-54	1178	202	10.1016/j.cej.2017.10.133
78	NiMoS chalcogels	490	225	10.1021/acs.chemmater.5b00413
79	MelPOP-2	50.5	262	10.1039/C8CC04242J
80	PSIF-1a	320	485	10.1021/acsami.8b03023

Sorption kinetics

Pseudo first order kinetic model

The linear form of pseudo first order kinetic model is expressed by the following equation.

$$\ln(q_e - q_t) = \ln q_e - k_1 t$$

Where q_e and q_t are the amount of iodine adsorbed at time t and equilibrium (g/g), k_1 is the pseudo-first-order rate constant of adsorption process(min^{-1})

Pseudo second order kinetic model

The linear form of pseudo second order kinetic model is expressed by the following equation.

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t$$

Where q_e and q_t are the amount of iodine adsorbed at time t and equilibrium (mg/g), k_2 is the pseudo-first-order rate constant of adsorption process (g/mg min)

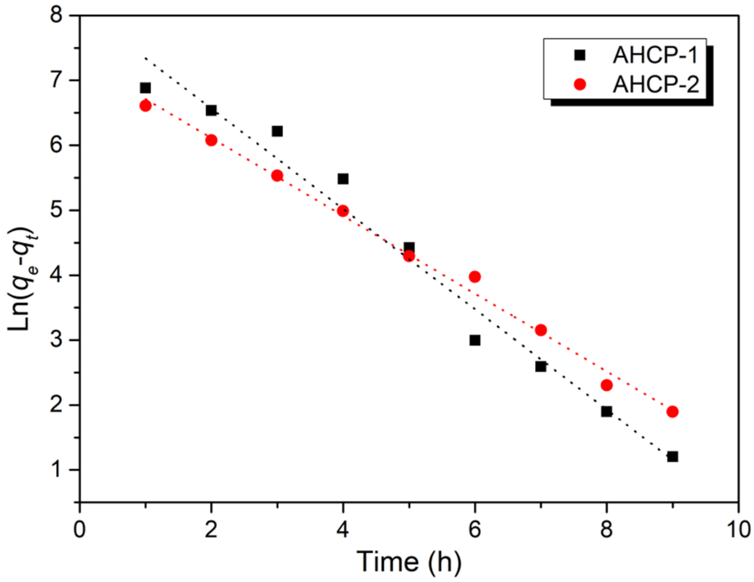

Fig. S3. Plots of pseudo-first order kinetics for the adsorption of I_2 aqueous solution on AHCP-1 and AHCP-2.

Table S3. Parameters of the pseudo first order and pseudo second order kinetic models extracted from experimental data for AHCP-1 and AHCP-2.

		Intercept	**q_e (g/g)**	**k_1(1/h)**	**R^2**
pseudo-first order	AHCP-1	8.1118	3.33	0.7729	0.9762
	AHCP-2	7.3119	1.49	0.5994	0.9939
		Intercept	q_e (g/g)	K_2(g/mg·h)	R^2
Pseudo second order	AHCP-1	0.0003	2.33	0.0006	0.9972
	AHCP-2	0.0006	1.67	0.0005	0.9990

Sorption equilibrium

Langmuir isotherm

The equation of Langmuir is expressed by the following equation.

$$\frac{1}{q_e} = \frac{1}{q_m} + \frac{1}{k_L q_m C_e}$$

Freundlich isotherm

The equation of Freundlich is expressed by the following equation.

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

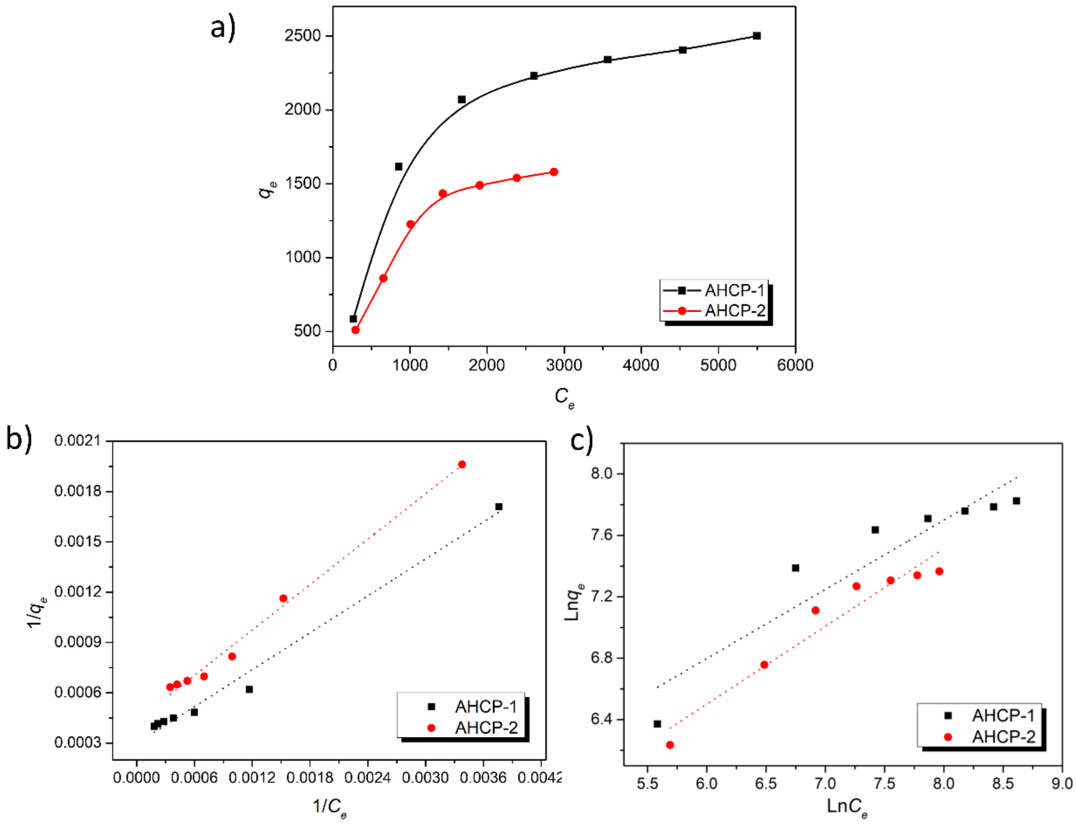

Fig. S4. (a) Adsorption Isotherm iodine onto AHCPs. (b) Plots of Langmuir Isotherms for the adsorption of I_2 aqueous solution on AHCP-1 and AHCP-2. (c) Plots of **Freundlich** Isotherms for the adsorption of I_2 aqueous solution on AHCP-1 and AHCP-2.

Table S4. Parameters of the different isotherm models extracted from experimental adsorption isotherms data for AHCP-1 and AHCP-2.

	Langmuir isotherm			Freundlich isotherm		
	Q_m(g/g)	k_L(1/mg)	R^2	k_F(mg/g)	n	R^2
AHCP-1	2.70	0.0011	0.9872	59.9074	2.2178	0.8766
AHCP-2	2.22	0.0010	0.9922	31.9317	1.9751	0.9330

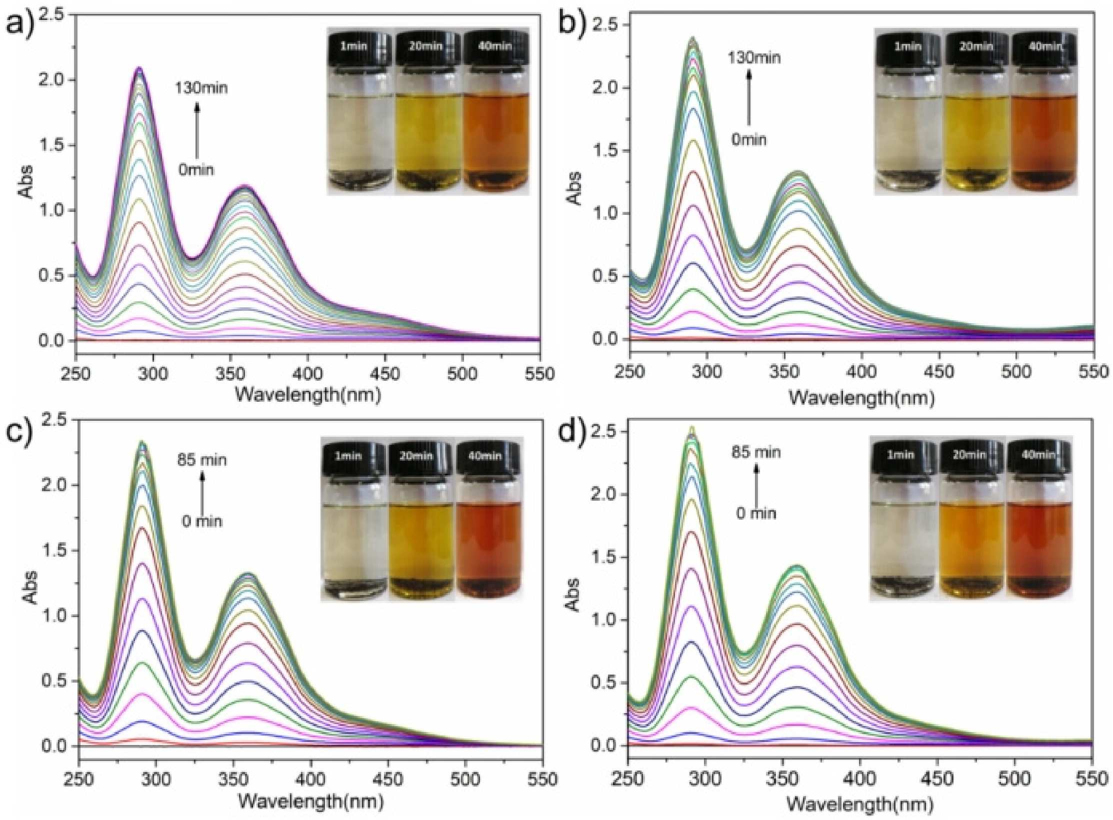

Fig. S5. Time-dependent UV−vis absorption of iodine@AHCPs in methanol. (a) iodine@AHCP-1(water) (10mg) in MeOH (45mL). (b) iodine@AHCP-2(water) (10mg) in MeOH (45mL). (c) iodine@AHCP-1(vapor) (10mg) in MeOH (80mL). (d) iodine@AHCP-2 (vapor) (10mg) in MeOH (80mL). Insets: photographs show color change of iodine enrichment at various times.

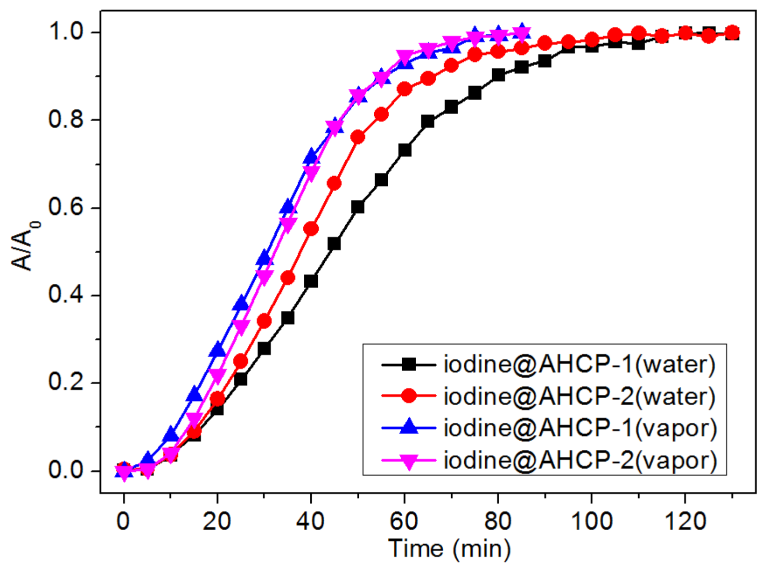

Fig. S6. Iodine desorption efficiencies at various times of iodine@AHCP-1(water), iodine@AHCP-2(water), iodine@AHCP-1(vapor), iodine@AHCP-2(vapor) monitored at 291nm.

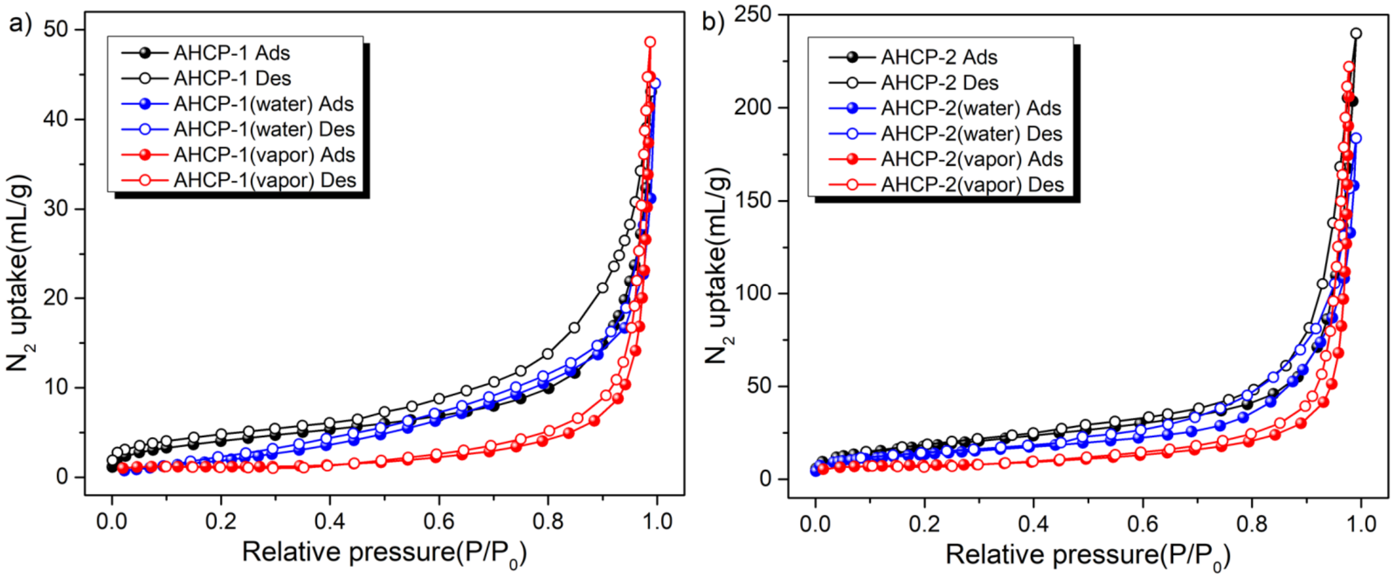

Fig. S7. BET curve after the first adsorption-desorption of iodine by AHCPs.

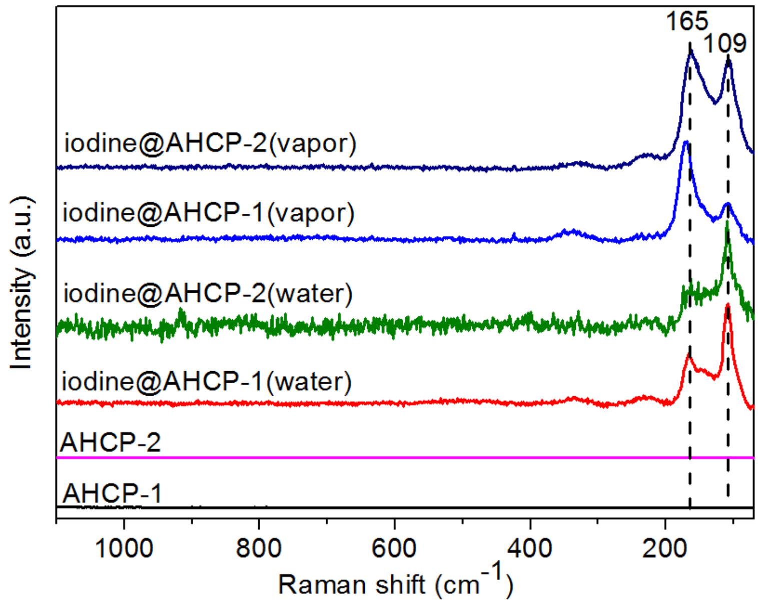

Fig. S8. Raman spectra of AHCPs, iodine@AHCPs(water) and iodine@AHCPs(vapor)

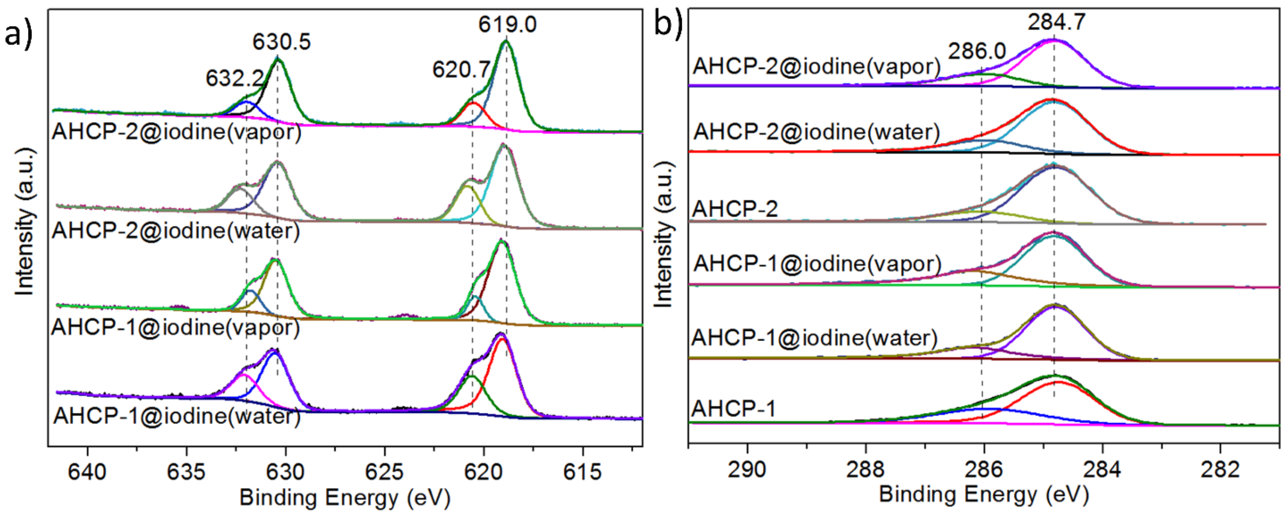

Fig. S9. XPS spectra of AHCPs, iodine@AHCPs(water) and iodine@AHCPs(vapor), (a) I3d; (b) C 1s,

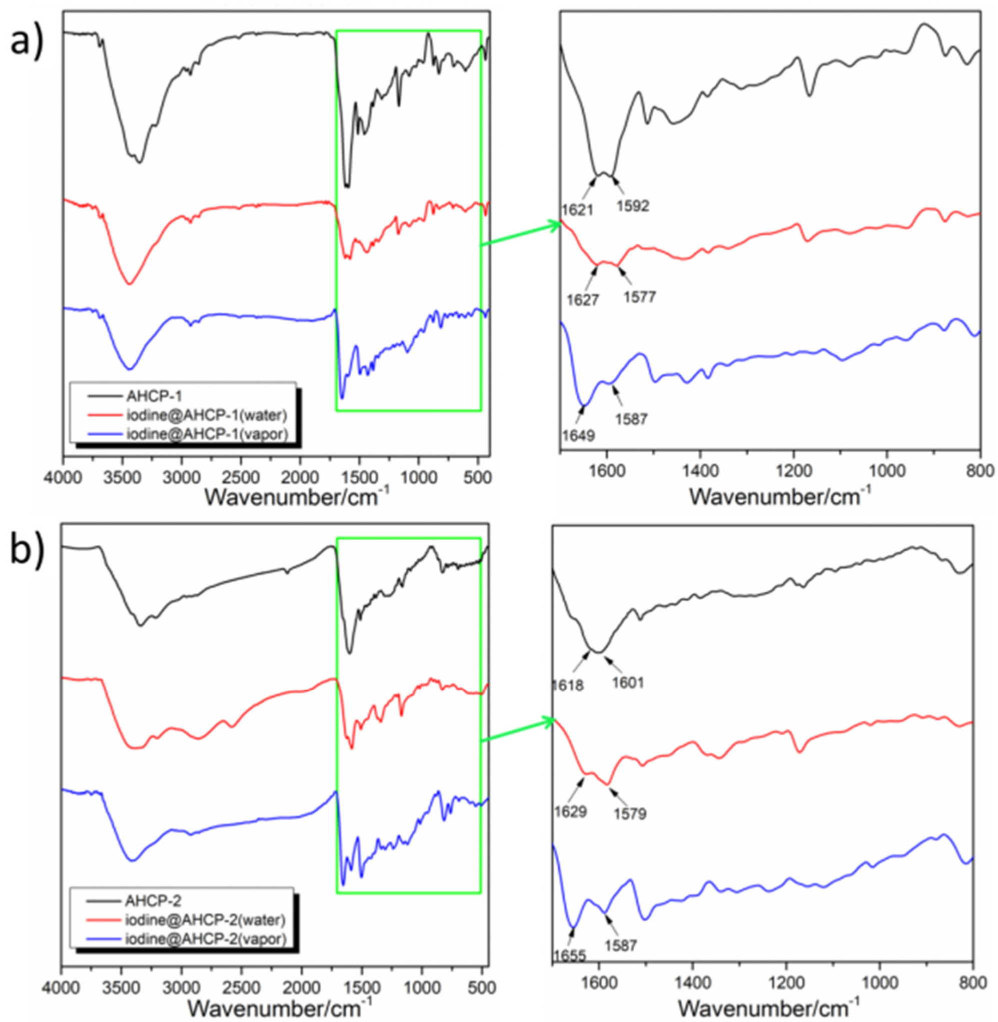

Fig. S10. (a) FT-IR spectra comparison of AHCP-1 before and after iodine adsorption; (b) FT-IR spectra comparison of AHCP-2 before and after iodine adsorption.