Super-Fast Iodine Capture by an Ionic Covalent Organic Network (iCON) from Aqueous and Vapor Medium

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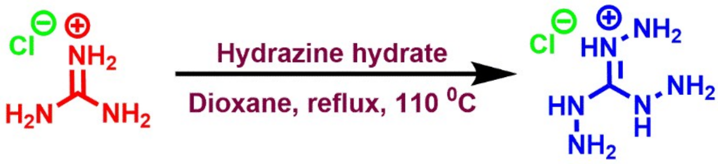
Experimental Section:

Synthesis of triaminoguanidium chloride (TAG_{Cl}):



Scheme S1. Synthesis of triaminoguanidinium chloride (TAG_{Cl})

To a mixture of 1.91 g (20 mmol) of guanidium hydrochloride, and 3.41 g (106 mmol) of hydrazine hydrate, 10 ml of 1, 4-dioxane was added under continuous stirring. The reaction mixture was refluxed for 2 hours. After that, the reaction mixture was allowed to cool down to room temperature and the product was filtered. Next, the product was washed with 1, 4-dioxane and dried to yield TAG_{Cl}.

Table S1: Solubility/insolubility chart of iCON-4

Organic Solvents	Solubility
Methanol	Insoluble
Dimethyl Sulfoxide	Insoluble
Dimethylformamide	Insoluble
Dimethylacetamide	Insoluble
Acetonitrile	Insoluble
1,2 – Dichloroethane	Insoluble
Tetrahydrofuran	Insoluble
Toluene	Insoluble
Xylene	Insoluble
Ethyl acetate	Insoluble
Hexane	Insoluble
Dichloromethane	Insoluble

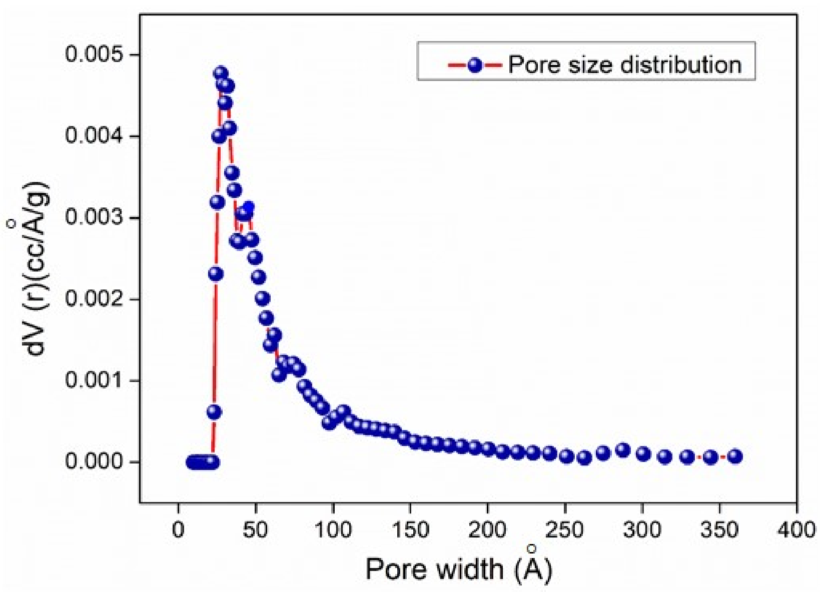


Figure S1 : NLDFT pore size distribution of iCON-4

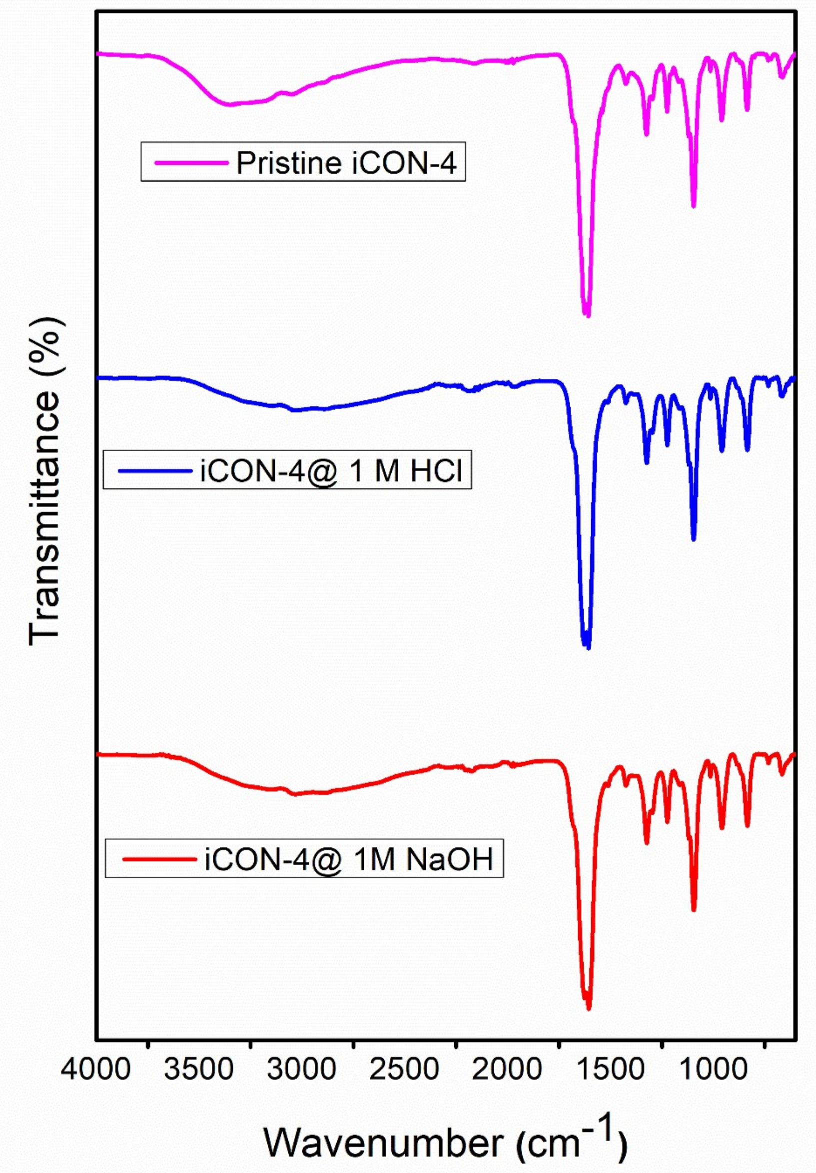


Figure S2. FTIR spectra of the iCON-4 along with acid and base treated iCON-4

Table S2: Comparison table of time required to remove iodine adsorbents from aqueous solution

Compounds	**Contact time**	**Selectivity**	**Recyclability**	**Ref**
iCON-4	**120 seconds**	**Cl^-,Br^-,NO_3^- ,SO_4^{2-}**	**7**	**This work**
CMP-4	180 min	NR	5	*Angew. Chem. Int. Ed.* 2021, 60,8967 –8975
Compound-1 Compound-2	10 min 30 min	Cl^-,Br^-,NO_3^- ,SO_4^{2-}	4	*ACS Appl. Mater. Interfaces* 2021, 13, 34188−34196

Nanobones, nanosheets	>78 mins	NR	NR	*ACS Appl. Mater. Interfaces* 2019, 11, 8537−8544
Cu-BTC@PES	>65min	NR	3	*ACS Appl. Mater. Interfaces* 2019, 11, 42635−42645
THPS-C	120 min	NR	5	*Adv. Mater. Interfaces* 2019, 1900249
TNHCPs	120 min	NR	5	*Separation and Purification Technology* 257 (2021) 117923
H_COF-1	240 min	NR	ND	*J. Am. Chem. Soc.* 2017, 139, 7172−7175
PTIBBL	500 min	NR	5	*Chem. Commun.,* 2020,56, 1401--1404
NTP	60 min	NR	5	*ACS Macro Lett.* 2016, 5, 1039−1043
MBM	>30 min	NR	NR	*Angew. Chem. Int. Ed.* 2018, 57,10148 –10152
SCNU-Z4	>960 min	NR	NR	*Inorg. Chem. Front.,* 2021, 8, 1083–1092
H_COF-3	240 min	NR	NR	*J. Am. Chem. Soc.* 2019, 141, 10915−10923

NR = Not reported

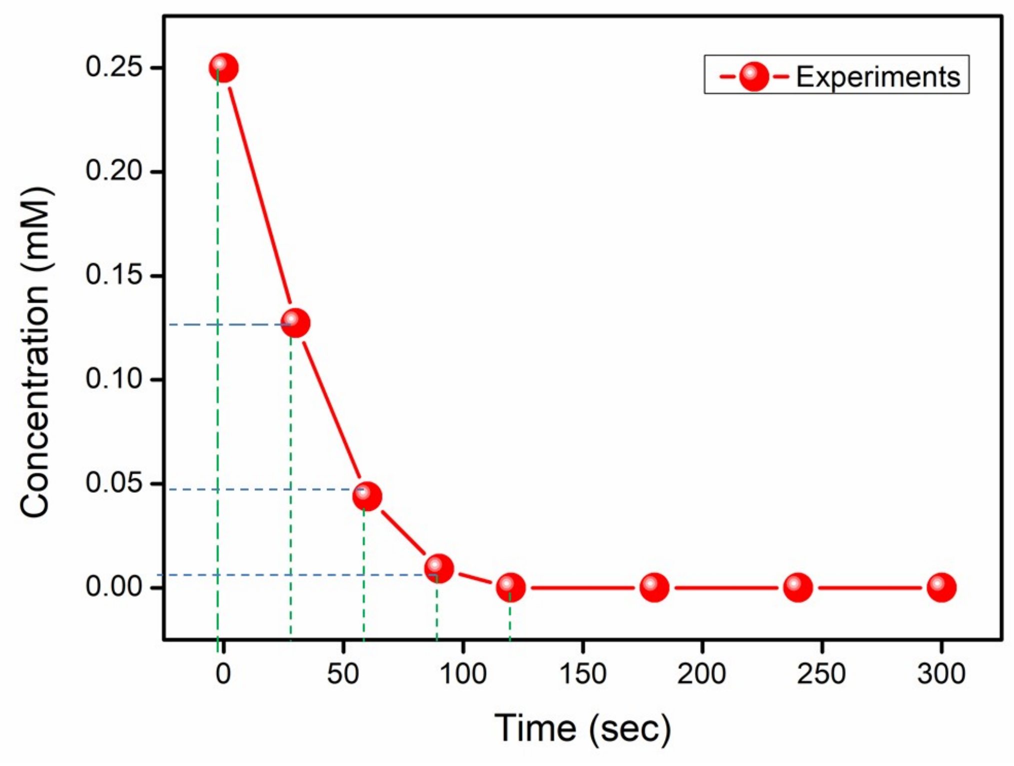


Figure S3. Change in concentration of iodine with time

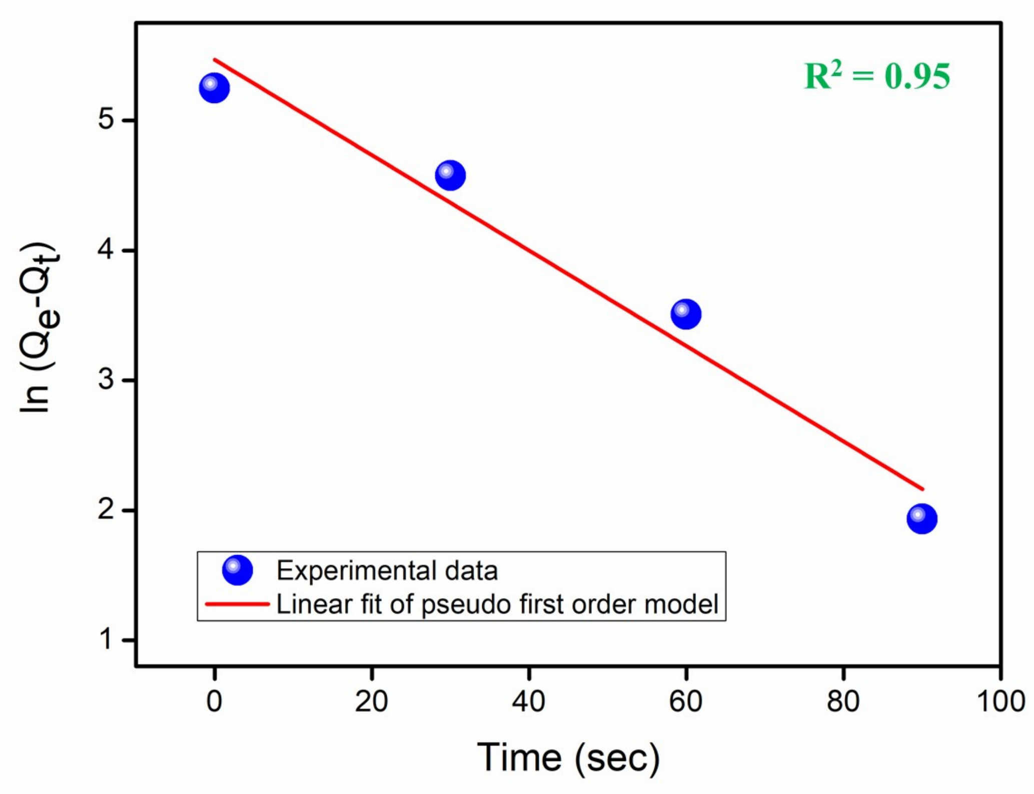


Figure S4. Pseudo first order data fitting of data related to adsorption of iodine by iCON-4 from aqueous solution

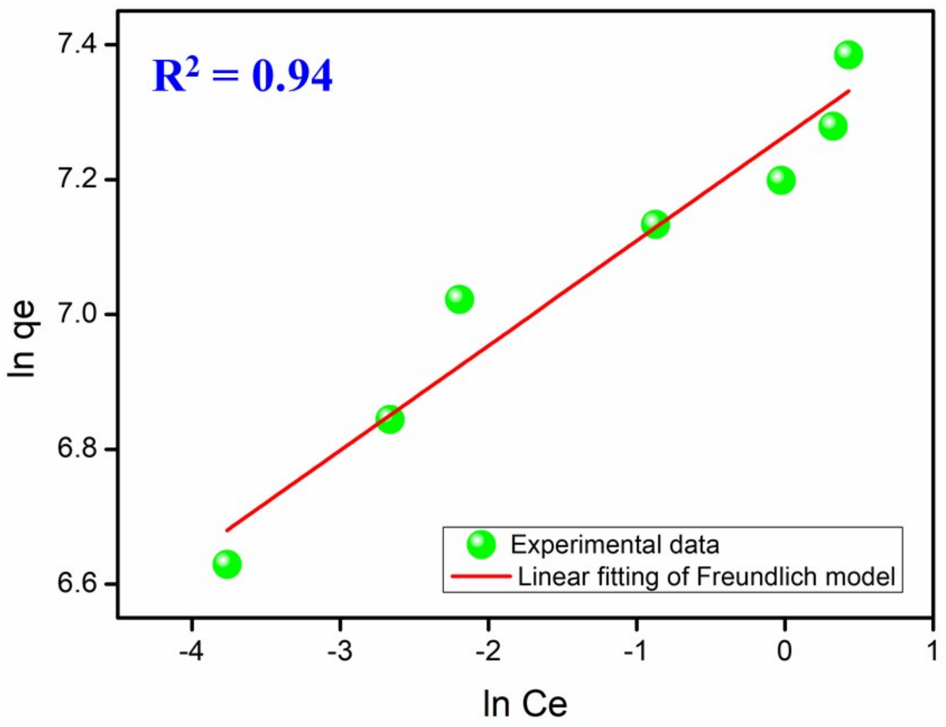


Figure S5. Fitting of iodine adsorption data of iCON-4 using the Freundlich isotherm model from water

Table S3: Comparison table of iodine capture by adsorbents from aqueous solution

Adsorbents	Medium	BET Suface area(m^2/g)	I_2 uptake (mg·g-1)	Reference
iCON-4	**Water**	**30.55**	**1632.17**	***This Work***
HcOF-1	Water	NR	2900	*J. Am. Chem. Soc.*, 2017, **139**, 7172−7175
Fe_3O_4@PPy	Water	NR	1627	*J. Hazard. Mater.*, **344** (2018) 576–584
PCN-223	Water	642.089	1615.882	*Sep. Purif. Technol.*, **233** (2020) 115999
PCN-223-HPP	Water	851.271	1676.960	*Sep. Purif. Technol.*, 233 (2020) 115999
{[$(ZnI_2)_3(TPT)_2$]·5.5 $(C_6H_5NO_2)$}n	Water	NR	1.73	Chem. Sci., 2017, 8, 3171
pSi–C composite	Water	762.13	299.40	*RSC Adv.*,2021,**11**,5268–5275
TAPB-BPDA COF	Water	1082	988.17	*React. Funct. Polym,* **159** (2021) 104806
THPS-C	Water	3125	926	*Adv. Mater. Inter.,* 2019, **6** , 1900249
NTP	Water	1067	429	*ACS Macro Lett.,*2016, **5**, 1039
Cadmium(II)-triazole	Water	NR	110	*Chem. Commun.,* 2011,**47**, 7185-7187

MOF				
MBM - MOF	Water	62	880	*Angew. Chem., Int. Ed.*, 2018, **57**, 10148
CdL2	Water	NR	460	Chem. Commun., 2011, **47**, 7185
PVDF/ZIF-8	Water	NR	73.33	*Sep. Purif. Technol.*, **238** (2020) 116488

NR= Not reported

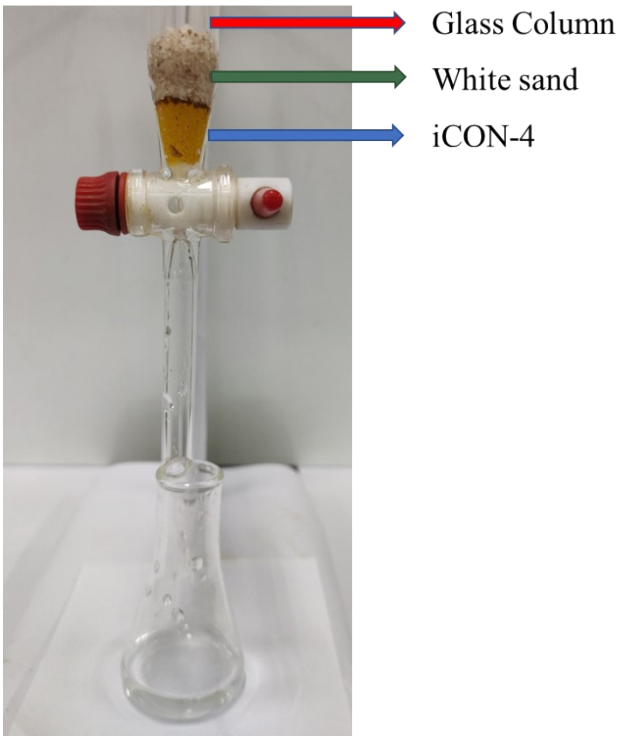


Figure S6. Column experiment setup for iodine adsorption by iCON-4

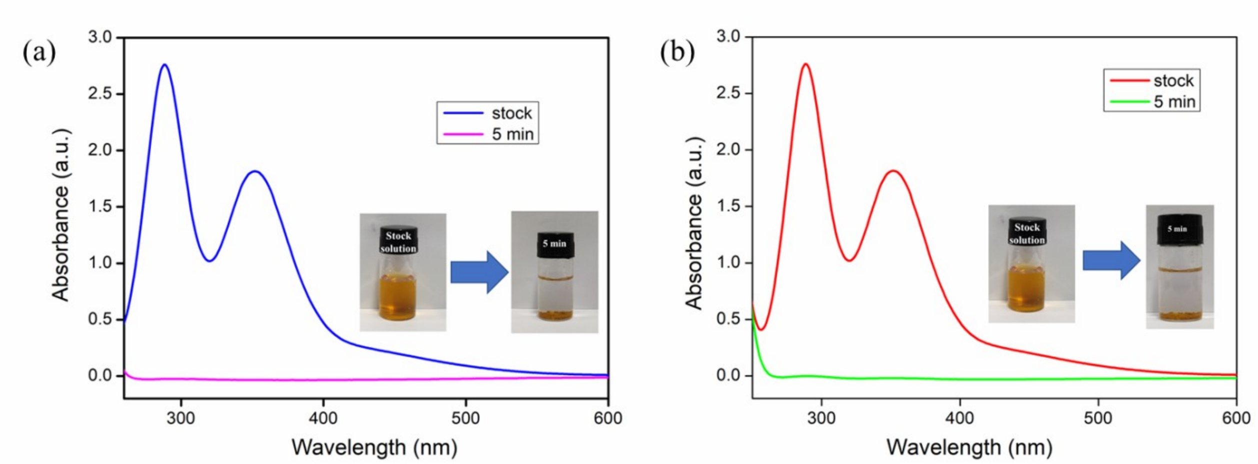


Figure S7. Iodine adsorption data of iCON-4 from iodine spiked (a) lake water (b) river water

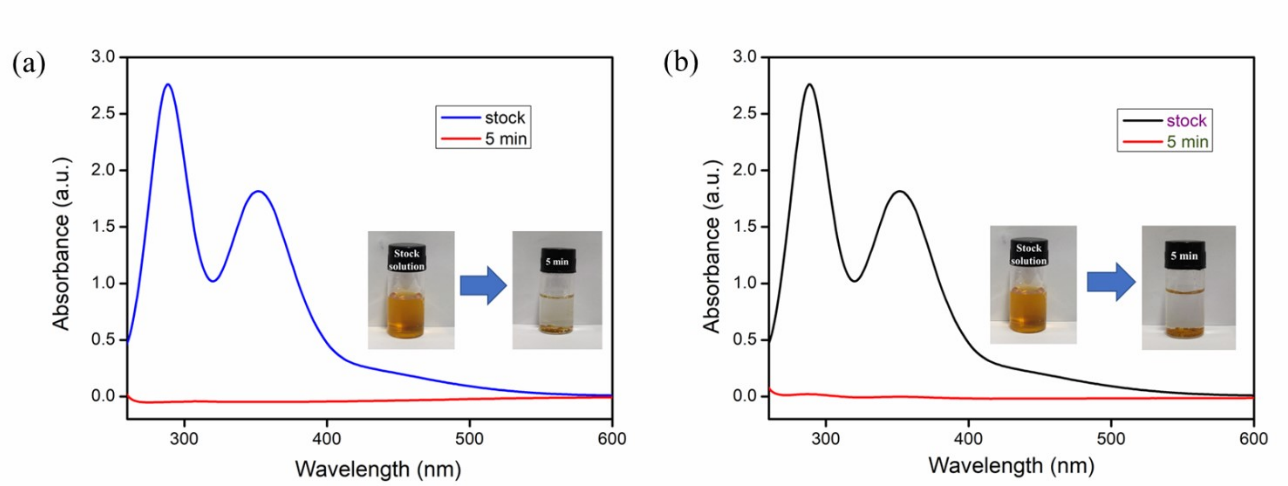


Figure S8. Iodine adsorption data of iCON-4 from iodine spiked (a) sea water (b) tap water

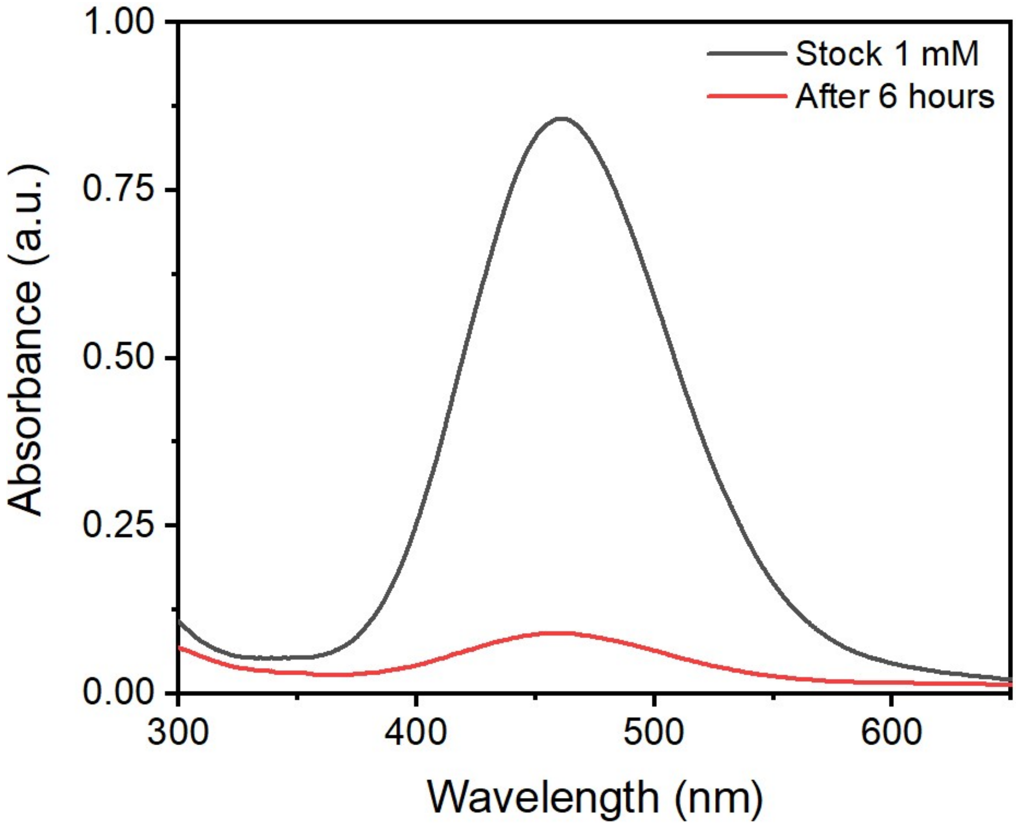


Figure S9. Adsorption data of iCON-4 for the capture of pure iodine from water.

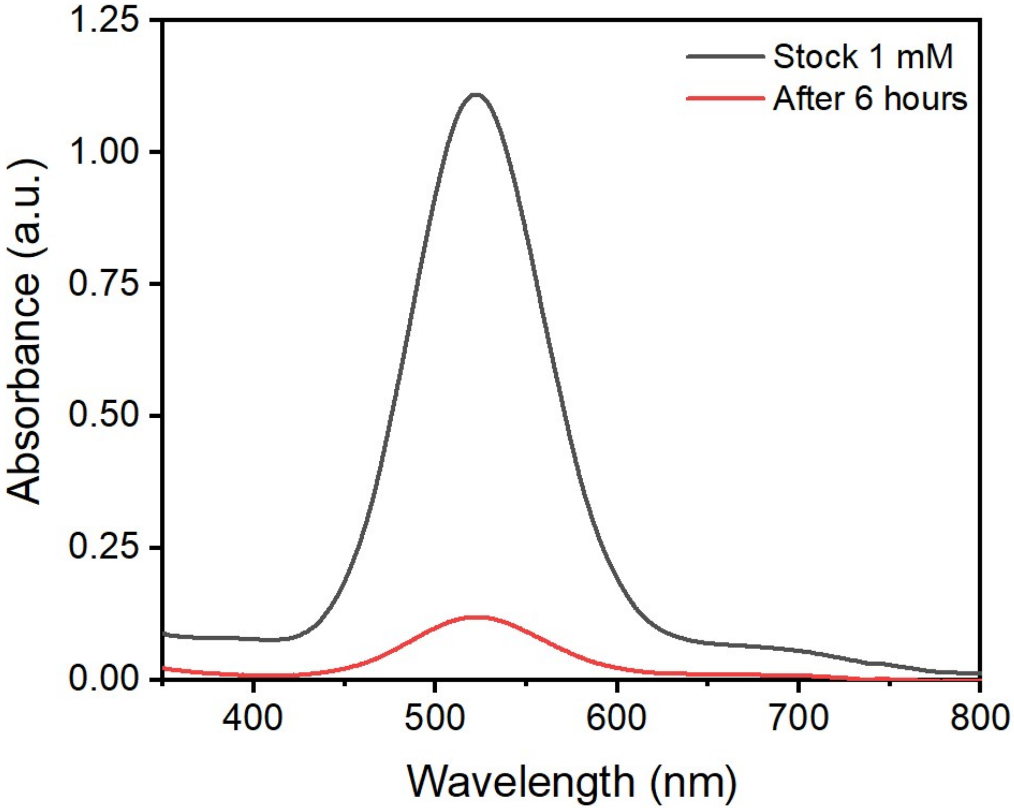


Figure S10. Iodine adsorption data of iCON-4 from n-hexane solution

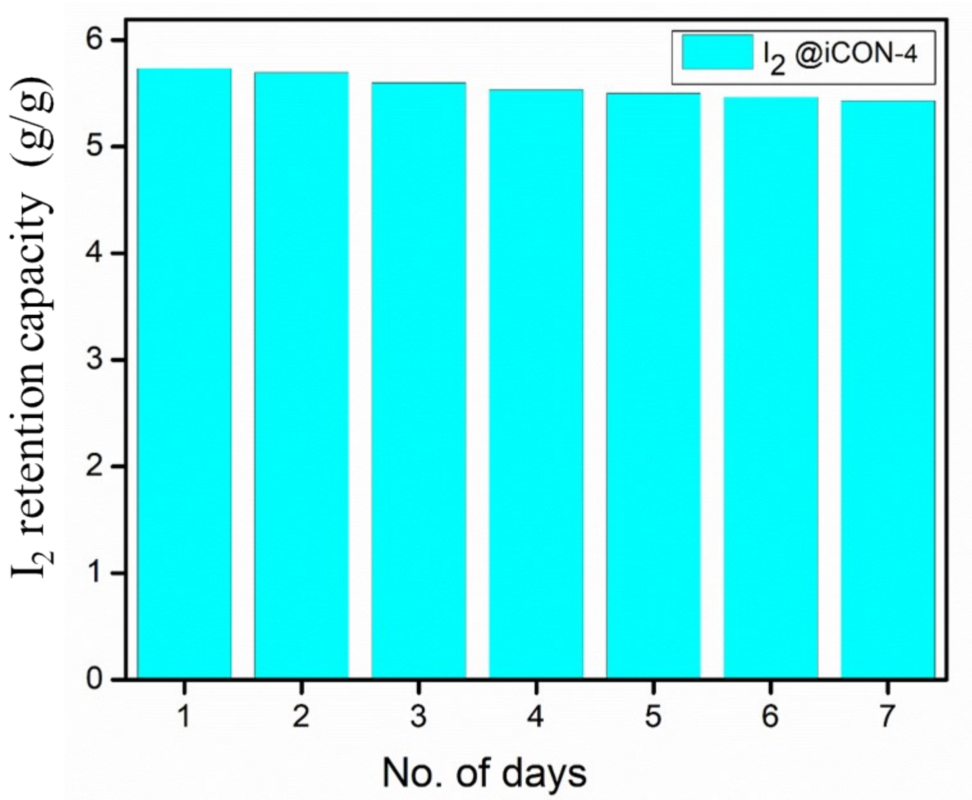


Figure S11. Retention capacity of I_2@iCON-4

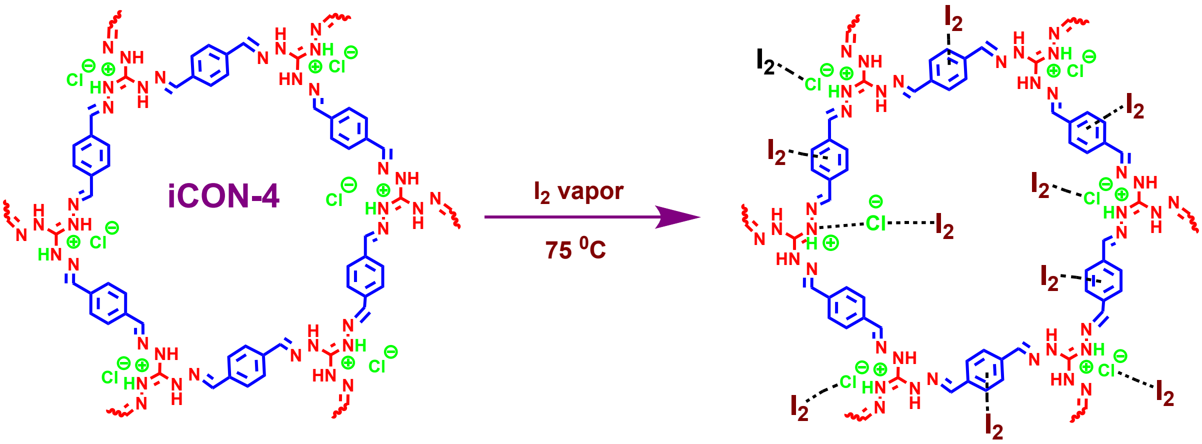


Figure S12. Probable schematic illustration of I_2 uptake mechanism by iCON-4 in vapor medium

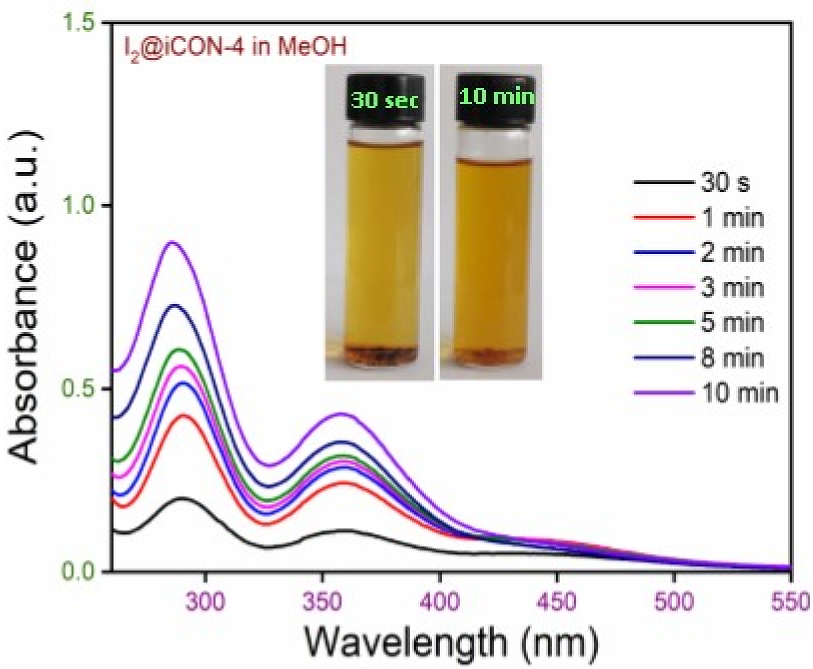


Figure S13. Iodine release in methanol from I_2@iCON-4

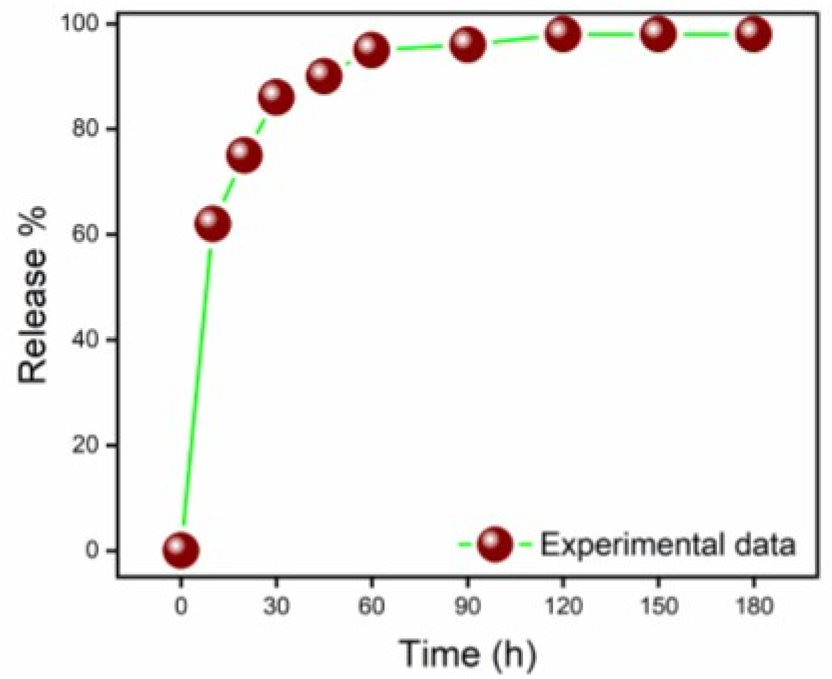


Figure S14. Iodine release from I_2@iCON-4 upon heating

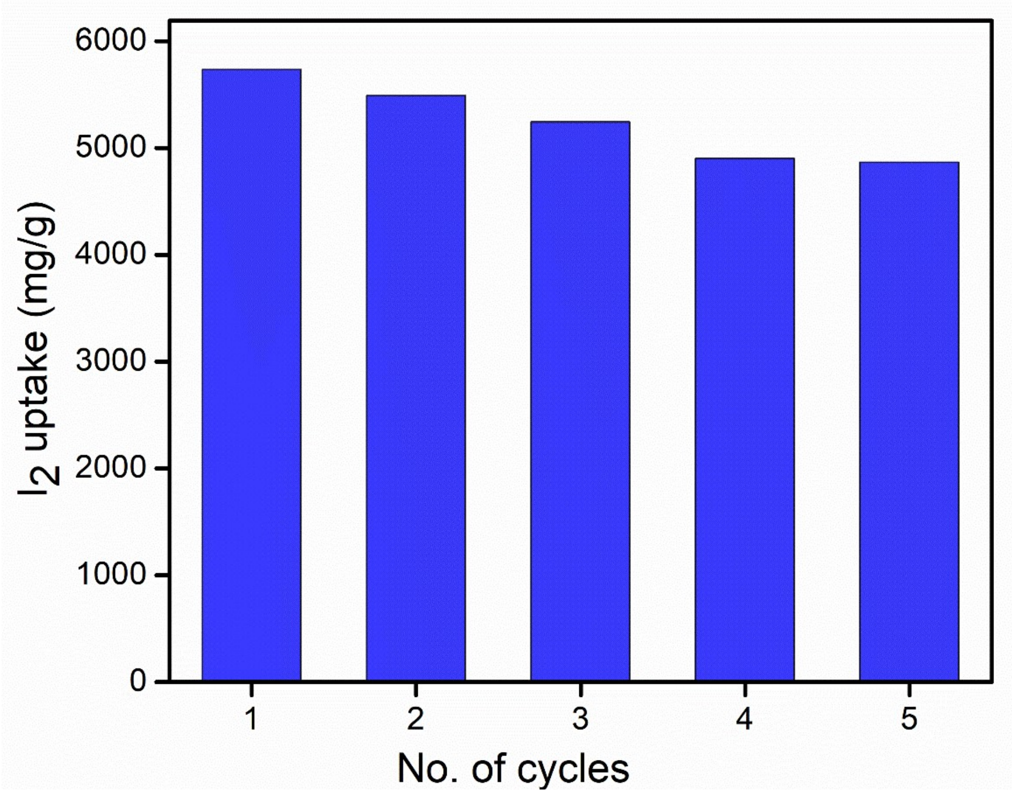


Figure S 15. Reusability of iCON-4 towards the iodine uptake in vapor phase

Table S4: Comparison table of iodine capture by adsorbents from vapor phase

Adsorbents	**Temperature (°C)**	**BET Suface area(m^2/g)**	**I_2 uptake (g·g-1)**	**Reference**
iCON-4	**75**	**30.55**	**5.7**	***This Work***
TPB-DMTP COF	75	1927	6.260	*Adv. Mater.*, 2018, **30**, 1801991
TBIM	77	8.12	9.43	*J. Mater. Chem. A,* 2020, **8**, 2820–2826
TJNU-201	77	2510	5.625	*J. Mater. Chem. A*, 2020, **8**, 9523-9527
NDB-H	75	117	4.430	*Chem. Asian J.*, 2018, **13**, 2046-2053
CMP-LS4	77	462	3.32	*Polym. Chem.***,** 2020, **11**,2786
PHF-1-Ct PHF-1	80	690 1046	4.05 3.05	*Chem. Commun.,* 2018,**54**, 12706-12709
CTF-CTTD-500	75	1334	3.87	*Ind. Eng. Chem. Res.*, 2018, 57, 44, 15114–15121
HCMP-3	75	92	3.36	*Macromolecules* 2016, 49, 17, 6322–6333
POP-1	80	12	3.570	*J. Hazard. Mater.*, 2017, **338**, 224-232

TBTT-CMP@3	77	62.89	3.52	*Polym. Chem.***,** 2020, **11**, 2786
Micro-COF-1 Micro-COF-2	75	816 1056	2.9 3.5	*Ind. Eng. Chem. Res.*, 2019, **58**, 10495-10502.
Azo-Trip	77	510.4	2.36	*Polym. Chem.,* 2016, **7**, 643
MOF-808	80	1930	2.18	*ACS Appl. Mater. Interfaces*, 2020, **12**, 20429–20439.
PAN-B PAN-T	75	1254 1273	3.17 3.11	*Polymer,* **194** (2020) 122401
PAF-24	75	136	2.76	*Angew. Chem. Int. Ed.,* 2015**, 54**, 12733–12737.
N-HCP	75	222.8	2.57	*Sep. Purif. Technol.,* **236** (2020) 116260
CMPNH2	75	6.44	2.83	*J. Mater. Chem. A*, 2020, **8**, 1966-1974.
CPP 1 CPP 2 CPP 3	80	NR	1.53 2.00 1.40	*Polym. Chem.***,** 2020, **11**,3066
PAN-FPP5 PAN-TPDA	71.85 71.85	788.0 752.0	1.45	*Ind. Eng. Chem. Res.*, 2020, **59**, 3269-3278.
NRPP-1 NRPP-2	80	1579 1028	1.92 2.22	*ACS Appl. Mater. Interfaces*, 2018, **10**, 16049-16058
CBP1 CBP2 CBP3 CBP4 CBP5	80	3.0 143 794 98 203	145 101 135 140 166	*Polym. Chem.***, 2021, 12,2282**
CMPN-3	70	1368	2.080	*J. Mater. Chem. A*, 2015, 3, 87-91.
HKUST-1	75	NR	1.75	*Chem. Mater.,* 2013, 25, 2591
ZIF-8	77	1630	1.250	*J. Am. Chem. Soc.,* 2011, 133, 12398-12401

NR = Not reported