

Supplementary Materials

The effect of pH on the adsorption of 2,4-dichlorobenzoic acid on carbon nanofibers produced via catalytic pyrolysis of tri-chloroethylene

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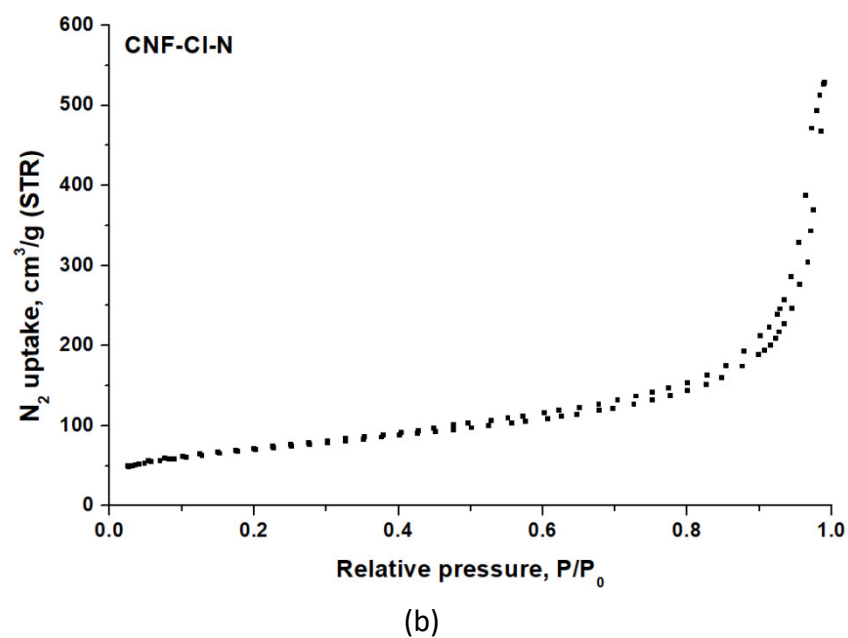
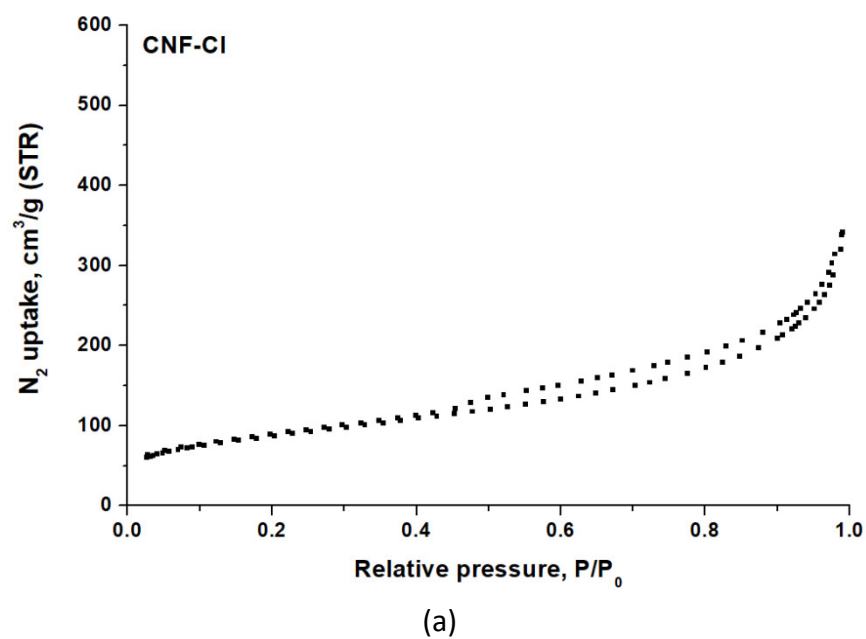


Figure S1. Nitrogen adsorption isotherm (77.4 K) for (a) CNF-Cl and (b) CNF-Cl-N.

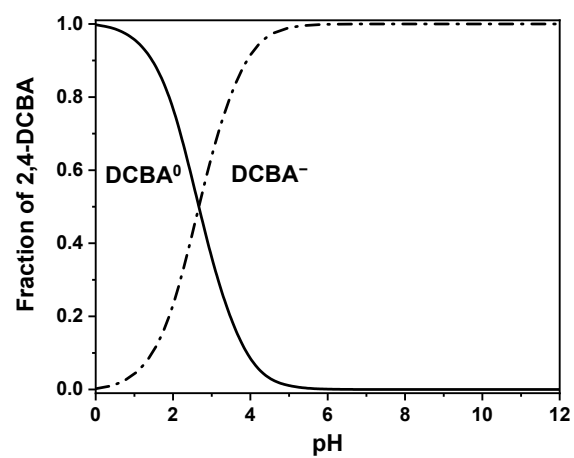


Figure S2. Species distribution of 2,4-DCBA as a function of solution pH.

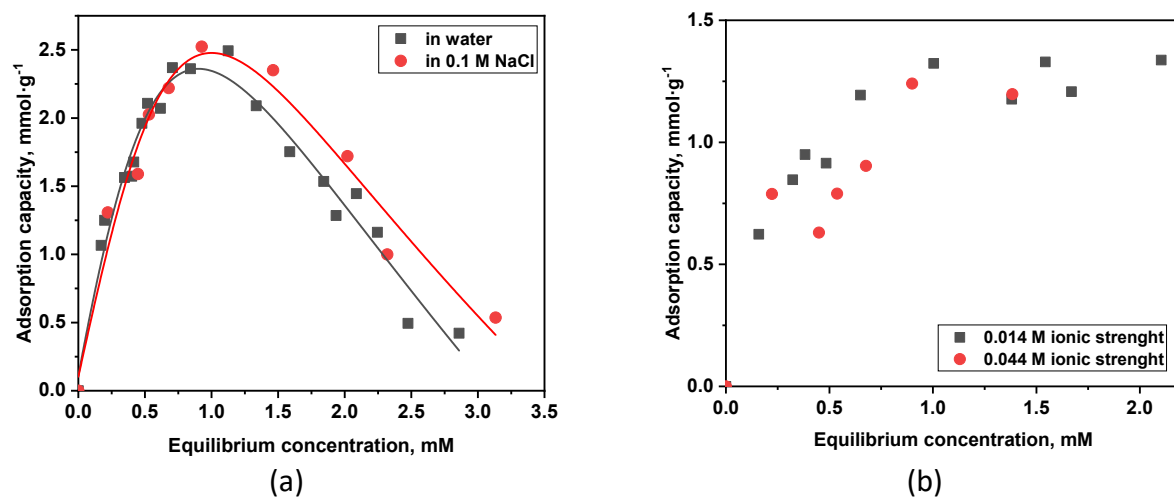


Figure S3. The influence of ionic strength on the adsorption of 2,4-DCBA on the carbon material. (a) Experimental adsorption isotherms of 2,4-DCBA obtained in water and 0.1 M NaCl solution at a natural pH. (b) Experimental adsorption isotherms of 2,4-DCBA at pH = 2 and different ionic strengths. Ionic strengths of 0.014 M and 0.044 M were obtained by using HCl with concentrations of 0.1 M and 2.45 M for adjusting the pH to 2.

Table S1. Values of parameters calculated from the Langmuir, Freundlich, and Dubinin–Astakhov adsorption isotherms for 2,4-DCBA on the CNF-Cl sample at different pHs.

Isotherm	Parameter	Value				
		pH=2	pH=3	pH=4	pH=5	pH=9
Langmuir	A_{\max} , mol·g ⁻¹	0.0024	0.0016	0.0014	0.0010	0.00022
	K_L , L·mol ⁻¹	2403	2901	1520	6409	13839
	R^2	0.984	0.934	0.977	0.943	0.990
Freundlich	K_F , mol·g ⁻¹	0.0016	0.0011	0.0008	0.0008	0.0002
	1/n	0.35±0.01	0.31±0.03	0.42±0.02	0.19±0.03	0.11±0.02
	R^2	0.999	0.959	0.983	0.968	0.992
Dubinin–Astakhov n=1	A_{\max} , mol·g ⁻¹	0.0021	0.0015	0.0012	0.0010	0.00021
	V_{\max} , cm ³ ·g ⁻¹	0.26	0.19	0.18	0.12	0.026
	$E_{\text{ads}}^{\text{eff}}$, kJ·mol ⁻¹	7.01	8.0	5.9	12.8	22.3
	R^2	0.999	0.959	0.983	0.968	0.992
Dubinin–Astakhov n=2	A_{\max} , mol·g ⁻¹	0.0019	0.0014	0.0010	0.00094	0.00021
	V_{\max} , cm ³ ·g ⁻¹	0.24	0.17	0.12	0.118	0.026
	$E_{\text{ads}}^{\text{eff}}$, kJ·mol ⁻¹	6.23	6.9	5.53	9.0	11.1
	R^2	0.968	0.918	0.957	0.943	0.990
Dubinin–Astakhov n=3	A_{\max} , mol·g ⁻¹	0.0018	0.0013	0.0010	0.00091	0.0002
	V_{\max} , cm ³ ·g ⁻¹	0.23	0.16	0.12	0.11	0.025
	$E_{\text{ads}}^{\text{eff}}$, kJ·mol ⁻¹	6.14	6.58	5.4	8.11	8.9
	R^2	0.916	0.876	0.906	0.913	0.985

Table S2. Values of parameters calculated from the Langmuir, Freundlich, and Dubinin–Astakhov adsorption isotherms for 2,4-DCBA on the CNF-Cl-N sample at different pHs.

Isotherm	Parameter	Value				
		pH=2	pH=3	pH=4	pH=5	pH=9
Langmuir	$A_{\max} \cdot \text{mol} \cdot \text{g}^{-1}$	0.0018	0.0010	0.00098	0.0008	0.00016
	$K_L \cdot \text{L} \cdot \text{mol}^{-1}$	1265	7570	3413	2205	10330
	R^2	0.960	0.965	0.971	0.929	0.954
Freundlich	$K_F \cdot \text{mol} \cdot \text{g}^{-1}$	0.00095	0.00087	0.00074	0.0005	0.00014
	$1/n$	0.49 ± 0.00	0.19 ± 0.03	0.32 ± 0.03	0.39 ± 0.04	0.12 ± 0.03
	R^2	0.988	0.981	0.977	0.947	0.943
Dubinin–Astakhov $n=1$	$A_{\max} \cdot \text{mol} \cdot \text{g}^{-1}$	0.0013	0.00099	0.00088	0.00066	0.00016
	$V_{\max} \cdot \text{cm}^3 \cdot \text{g}^{-1}$	0.16	0.12	0.11	0.084	0.02
	$E_{\text{ads}}^{\text{eff}} \cdot \text{kJ} \cdot \text{mol}^{-1}$	5.0	12.58	7.73	6.34	20.0
	R^2	0.988	0.981	0.977	0.947	0.956
Dubinin–Astakhov $n=2$	$A_{\max} \cdot \text{mol} \cdot \text{g}^{-1}$	0.0011	0.0009	0.0008	0.00059	0.00015
	$V_{\max} \cdot \text{cm}^3 \cdot \text{g}^{-1}$	0.14	0.11	0.10	0.07	0.019
	$E_{\text{ads}}^{\text{eff}} \cdot \text{kJ} \cdot \text{mol}^{-1}$	5.02	8.7	6.34	5.8	10.4
	R^2	0.902	0.961	0.958	0.905	0.952
Dubinin–Astakhov $n=3$	$A_{\max} \cdot \text{mol} \cdot \text{g}^{-1}$	0.0010	0.00088	0.00075	0.00056	0.00015
	$V_{\max} \cdot \text{cm}^3 \cdot \text{g}^{-1}$	0.125	0.11	0.094	0.07	0.019
	$E_{\text{ads}}^{\text{eff}} \cdot \text{kJ} \cdot \text{mol}^{-1}$	5.19	7.9	6.12	5.7	8.4
	R^2	0.820	0.942	0.920	0.840	0.956

Table S3. Comparison of maximum adsorption capacities of various adsorbents for 2,4-DCBA.

Adsorbent	Concentration range of 2,4-DCBA, mM	Sorbent dosage, mg/mL	Contact time, hr	pH	Maximum adsorption capacity, mmol/g	Reference
Pd/CB	0-0.275	0.4	3	4	0.26	[1]
Pd/MWCNTs					0.16	
Pd/GAC					0.05	
CTAB-Pd/GAC	0-0.0156	1	3	not mentioned	0.013	[2]
CNF-Cl	0-2.5	0.05	24	natural	2.32	This work
CNF-Cl-N					2.29	

CB: carbon black; MWCNTs: multi-walled carbon nanotubes; GAC: granular activated carbon; CTAB-Pd/GAC: functionalized palladium/granular activated carbon with cetyltrimethylammonium bromide.

1. Zhou, J.; Lou, Z.; Yang, K.; Xu, J.; Li, Y.; Liu, Y.; Baig, S.A.; Xu, X. Electrocatalytic Dechlorination of 2,4-Dichlorobenzoic Acid Using Different Carbon-Supported Palladium Moveable Catalysts: Adsorption and Dechlorination Activity. *Appl. Catal. B Environ.* **2019**, *244*, 215–224, doi:10.1016/j.apcatb.2018.11.052.
2. Zhou, J.; Lou, Z.; Wang, Z.; Zhou, C.; Li, C.; Ali Baig, S.; Xu, X. Electrocatalytic Dechlorination of 2,4-DCBA Using CTAB Functionalized Pd/GAC Movable Granular Catalyst: Role of Adsorption in Catalysis. *Chem. Eng. J.* **2021**, *414*, 128758, doi:10.1016/j.cej.2021.128758.