Supplementary Material

Cyclodextrin-silica hybrid materials: synthesis, characterization, and application in pesticide aqueous removal

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Table S1. CP/MAS ^{13}C NMR (δ/ppm) for cyclodextrins (α and γ) free and functionalized.

	C-1	*C-4*	*C-2,3,5*	*C-6*	*Esther and/or carboxylic acid*	*CH_2 (ligand)*
α-CD	103.78	85.33	75.78	61.70		
	103.21	83.00	74.78	61.14		
	102.87	81.88	74.25			
	101.99	80.56	73.63			
	98.07	77.71	73.01			
			72.31			
			71.65			
mean	102.87	81.88	73.63	61.42		
α-CDSi	102.22	81.53	73.39	64.62	172.93	43.43
γ-CD	105.09	84.60	75.11	64.49		
	103.96	83.33	74.11	63.15		
	103.38	82.52	73.58	61.02		
	102.18	81.99	73.33	60.11		
	101.35	81.41	72.29			
	101.12	79.58	71.47			
	99.85	78.61	71.01			
	98.91	77.49				
	98.17	76.74				
mean	101.35	81.41	73.33	63.15		
γ-CDSi	102.63	82.31	73.97	64.91	173.1	44.20

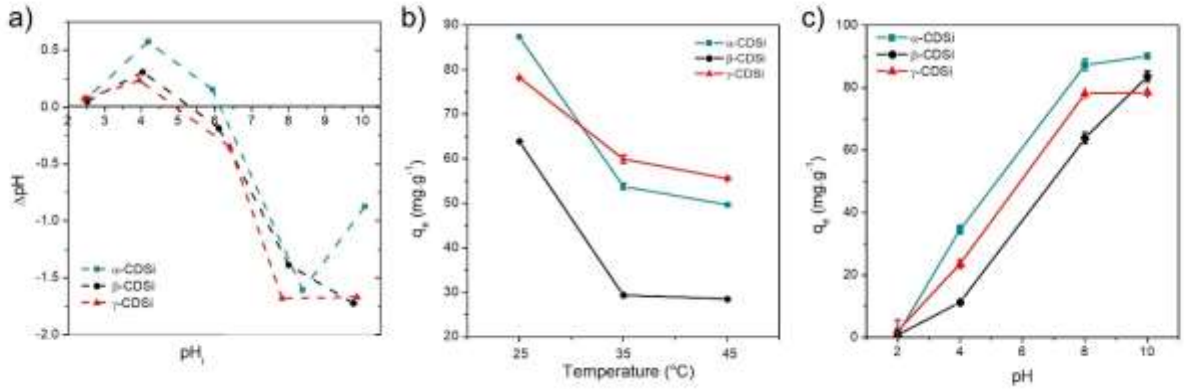

Figure S1. (a) PZC determination in CDSi composites samples: α-CDSi, β-CDSi, and γ-CDSi. (b) Temperature and (c) pH effect on the PQ adsorption ($[PQ]_0$= 20 mg.L^{-1}, adsorbent dose = 0.02 %w/v).

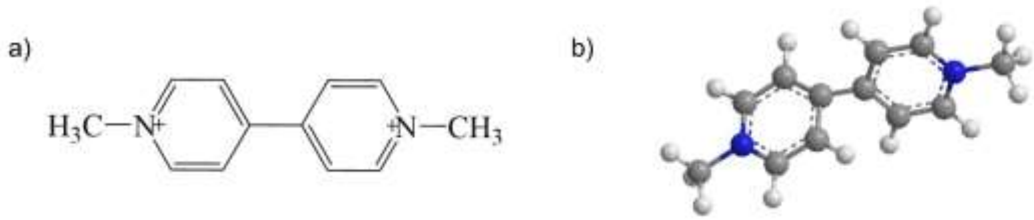

Figure S2. PQ structure (a) 2D, and (b) 3D.

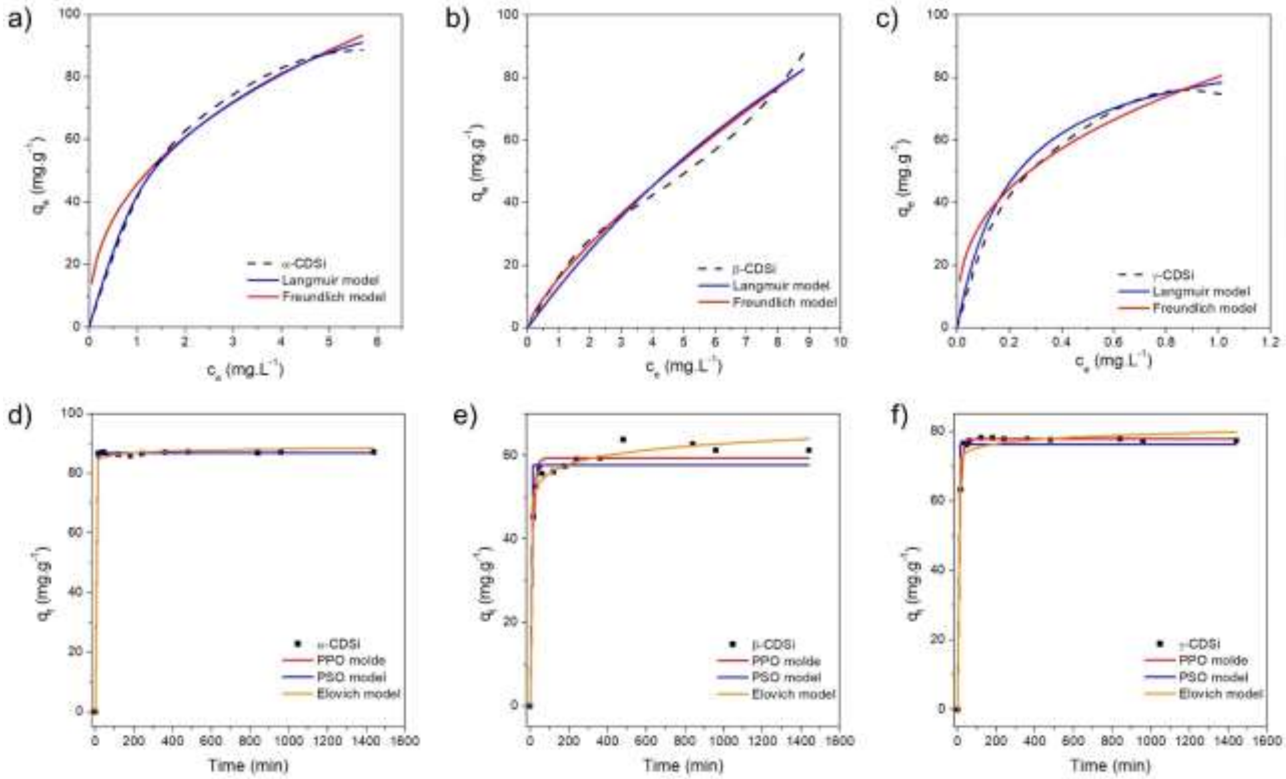

Figure S3. Non-linear fitting of PQ adsorption experimental data to the Langmuir and Freundlich isotherm models to the (a) α-CDSi, (b) β-CDSi, and (c) γ-CDSi composites. PFO, PSO and Elovich kinetic models to the (d) α-CDSi, (e) β-CDSi, and (f) γ-CDSi composites.

Table S4. Performance comparison of various PQ adsorption parameters reported for different CD and other materials reported: q_e, equilibrium removal time, temperature, mechanism, and dosage of PQ and adsorbent.

Materials	*q_e (mg.g^{-1})*	*C_o (mg.L^{-1})*	*Dose (%w/v)*	*T° (°C)*	*pH*	*S_{BET} (m^2.g^{-1})*	*Equilibrium time (min)*	*M#*	*Reference*
CD MATERIALS									
β-cyclodextrin and 1,2,3,4-butanetetracarboxylic acid	10.8	25	0.2	30	8	0.15	120	L	(Junthip et al., 2019)
	19.7	50	0.2	30	8	0.15	120	L	(Junthip et al., 2019)
	25.8	200	0.2	30	8	0.15	120	L	(Junthip et al., 2019)
Cyclodextrin polymer crosslinked with citric acid	9.4	25	0.2	30	6.5	0.63	120	L	(Junthip, 2019)
	17.4	50	0.2	30	6.5	0.63	120	L	(Junthip, 2019)
	20.8	200	0.2	30	6.5	0.63	120	L	(Junthip, 2019)
	5	10	0.2	30	8	n.r.	360	L	(Junthip et al., 2018)

PET textiles coated with anionic cyclodextrin polymer	20.4	50	0.2	30	8	n.r.	360	L	(Junthip et al., 2018)
	25.9	250	0.2	30	8	n.r.	360	L	(Junthip et al., 2018)
Textile coated with anionic cyclodextrin polymer	4.5	10	0.2	30	6.5	n.r.	360	L	(Junthip et al., 2018)
	18.9	50	0.2	30	6.5	n.r.	360	L	(Junthip et al., 2018)
	23.7	250	0.2	30	6.5	n.r.	360	L	(Junthip et al., 2018)
Poly(vinyl alcohol)-cyclodextrin nanosponges	10.6	25	0.2	30	6.5	0.176	60	L	(Martwong et al., 2021)
b -Cyclodextrin nanosponges cross-linked with 1,2,3,4-butanetetracarboxylic acid and poly(vinyl alcohol)	12	25	0.2	30	8	n.r.	100	L	(Martwong et al., 2022a)
Cotton cord coated with 10 % b -cyclodextrin polymers	4.56	25	0.5	30	8	n.r.	200	L	(Martwong et al., 2022b)

Cotton cord coated with 5 % b-cyclodextrin polymers	4.75	25	0.5	30	8	n.r.	200	L	(Martwong et al., 2022b)
α-CDSi	**87.36**	**25**	**0.02**	**25**	**8-10**	**80**	**30**	**L-F**	**This work**
β-CDSi	**63.88**	**25**	**0.02**	**25**	**8-10**	**76**	**60**	**n.r.**	**This work** (Bragança Carvalho et al., 2019)
γ-CDSi	**78.19**	**25**	**0.02**	**25**	**8-10**	**26**	**30**	**L-F**	**This work**
OTHER MATERIALS									
Bentonite/zero valen iron	6.78	20	0.24	25	10	n.r.	1440	L	(Dehgani et al., 2020)
NaY Zeolite	234.4	1500	0.25	25	7	798	1440	L	(Rongchapo et al., 2017)
Carbon tubes	218.61	500	0.04	20	10	43.86	20	L	(Li et al., 2021)
Graphene oxide/mesoporous silica	29.15	24	0.08	25	7	134.33	1440	L	(Dehghani et al., 2021)
Bentonite/mesoporous silice	11.75	8	0.16	25	7	15.21	1440	L	(Rasaie et al., 2021)

Fe_3O_4@SiO_2@SBA-3-SO_3H	80	75	0.24	25	7	70.42	120	L	(Kouchakinejad et al., 2022)
FJS/InMOF	56.03	12	0.3	25	n.r.	n.r.	720	n.r.	(Sun et al., 2022)

[#]M: mechanism

*n.r.: non reported

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