SUPPORTING INFORMATION

Polyethersulfone Nanofibers impregnated with β-Cyclodextrin for increased Micropollutant Removal from Water

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Supporting information 1: Summary of previous studies on incorporation of CD to electrospun nanofibers for adsorption of organic molecules

Table S1. Summary of previous studies on incorporation of CD into electrospun nanofibers for adsorption of organic molecules

Nanofiber material	CD type	CD in fibers (%w/w)	CD incorp. method	Fiber diameter (nm)	Adsorbed molecule	Filtration method	Maximum removal	Target application	Ref.
Poly (methyl methacrylate) (PMMA)	α, β, ɣ	5-50	Blending	625 -1024	–	–	–	Molecular filters and/or nanofilters for waste treatment	1
Polystyrene (PS)	Β	10-50	Blending	1161-1959	Phenolphthalein	Batch adsorption	~65% after 3 days	Filtration of organic molecules in purification/separation	2
Regenerated cellulose	α, β, ɣ	4-10	Blending and grafting	227-506	Toluene	Batch adsorption	82% after 180 min	Wastewater treatment	3
Poly (acrylonitrile-acrylic acid) (PANAA)	Β	10-100	Blending	231-620	Phenol-phthalein	Batch adsorption	80% after 10 min	Filtration/purification/separation purposes	4
Polystyrene (PS)	α, β, ɣ	21.3, 25, and 28.5	Blending	940-1959	Phenol-phthalein	Batch adsorption	80% after 72 h	Filtration, purification, and/or separation processes	5
Poly (vinyl alcohol) (PVA)	Β	10-40	Blending	170-260	ferrocene (Fc)	Batch adsorption	–	Recognition of small hydrophobic molecules such as ferrocene (Fc)	6
Polystyrene (PS)	α, β, ɣ	1-3	Blending	–	Cu (II)	Batch adsorption	35% after 14 h	Functional fibrous materials in aqueous solution	7
Zein	α, β, ɣ	10, 25 and 50	Blending	~100–400	–	–	–	–	8
Polystyrene (PS) fibers coated with Polydopamine (PDA)	Β	1.8	Surface attachment (PDA+CD)	–	Phenolphthalein (highly basic conditions)	Batch adsorption	~8.7 mg/g for 24 h	Water purification	9
Polyvinyl alcohol (PVA)/SiO2/ tetraethyl orthosilicate (TEOS)	silylated monochlorotriazinyl β –CD	30	Sol–gel/electrospinning process	200-300	Indigo carmine dye	Batch adsorption	495 mg/g in 40 min	Dye removal	10
Poly (L-lactide) (PLLA) and poly (D-lactide) (PDLA)	Mono-6-deoxy-(p-tolylsulf-onyl)-β-cyclodextrin (CD-O-Ts)	–	Surface attachment (grafting reaction)	1000	Alizarin red	Batch adsorption	12 (mg /g)	Absorb water pollutants	11
					2-chlorophenol		42 (mg /g)		
Polyester (PET)	α, β, ɣ	10	Surface modification (cross linked with citric acid)	870-1290	Polycyclic aromatic hydrocarbon (PAH)	Batch adsorption	~83 % after 30 h	Water purification and waste treatment	12

Cellulose acetate (CA)	azide- β-CD	–	Click reaction (Grafting of azide- β-CD onto CA nanofibers)	675 -1520	Phenan-threne (polycyclic aromatic hydrocarbons,PAH)	Batch adsorption	95% after 14 h	Water purification and waste water treatment	13
Poly (acrylic acid) (PAA)/citric acid	B	15.6	Blending (cross linked)	–	Methylene blue	Batch adsorption	～93% after 5 cycles	Dye wastewater treatment	14
						Dynamic adsorption	～90% after 5 cycles		
poly (vinyl alcohol) (PVA)/ sericin/citric acid	B	1.14	Blending	–	Methylene blue	Batch adsorption	92.60% after 5 cycles	Dye wastewater treatment	15

Supporting Information 2: Modelling of adsorption kinetics using first and second order kinetic models

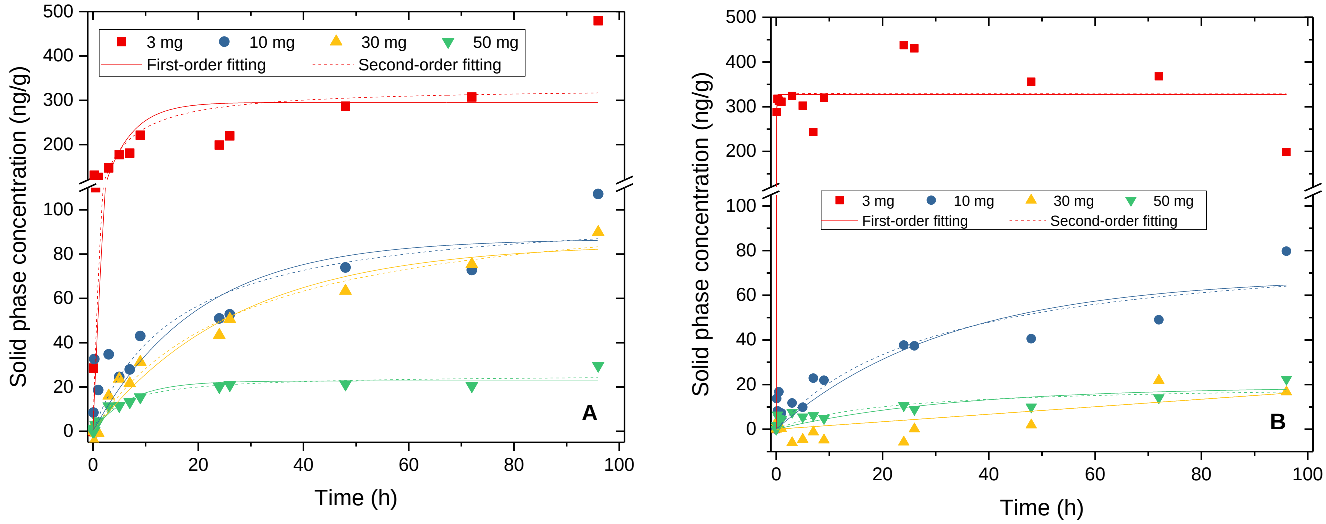

Figure S1. Adsorption kinetics displayed by PES (A) and PES+CD (B), with first-order kinetic model fitting (solid line) and second-order kinetic model fitting (dashed line).

Table S2. Comparison between pseudo first- and second-order kinetic models for the characterization of E2 adsorption by PES and PES+CD.

Model	**Formula**	**Eq.**	**Units**	**Ref.**
Pseudo first-order	$q_t = q_e.(1 - e^{-K_1.t})$	(5)	$K_1 = \mathrm{h}^{-1}$	16
Pseudo second-order	$\frac{1}{q_t} = \frac{1}{K_2 {q_e}^2}\frac{1}{t} + \frac{1}{q_e}$	(6)	$K_2 = \mathrm{g.ng^{-1}.h^{-1}}$	

In which, t is the adsorption time (h), q_t is the solid phase concentration of E2 (ratio of mass of E2 mass of adsorbent) at time t (ng/g); q_e is the solid phase concentration of E2 at equilibrium (ng/g); K_1 and K_2 are the first- and second-order kinetic rate constants, respectively.

Supporting information 3: TG-curves of PES and PES+CD nanofiber after 24 h in MilliQ water

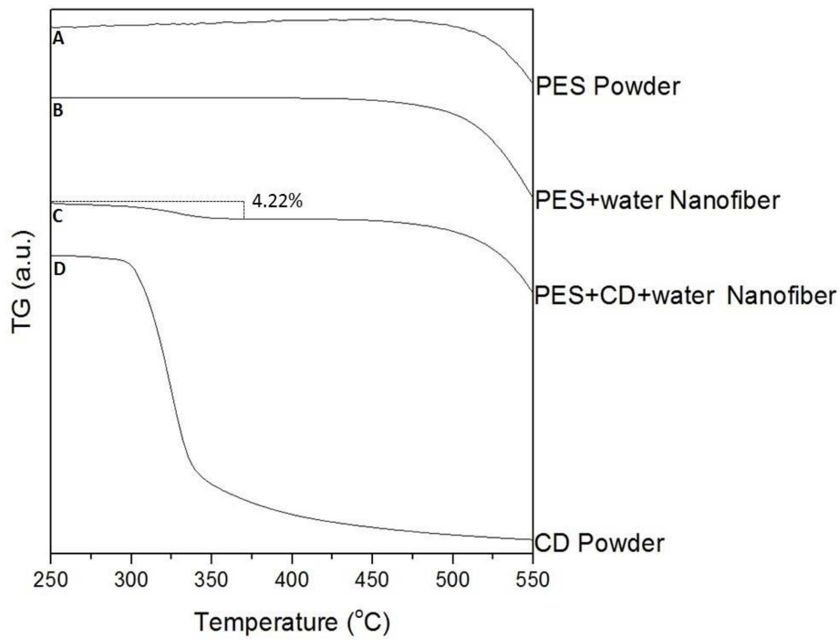

Figure S2. TG-curves of A) Pure PES powder, B and C) PES and PES+CD nanofiber after 24 h shaking at 260 rpm in 100 mL of MilliQ water at 20 °C, D) Pure cyclodextrin (CD) powder.

Supporting information 4: MS-curves of CO_2 (m/z =44)

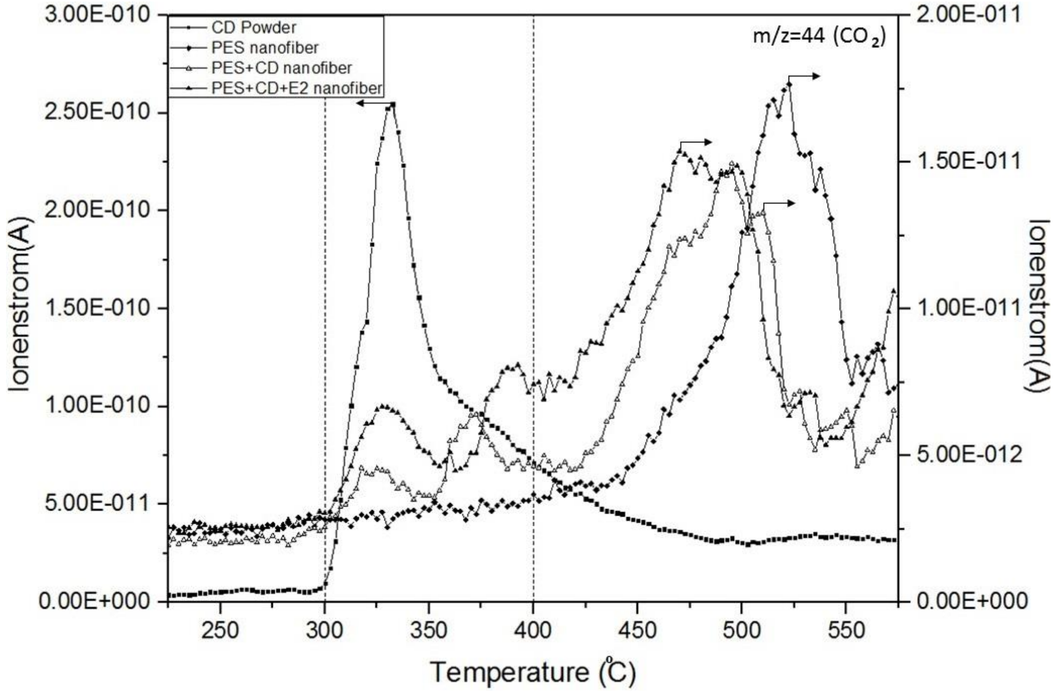

Figure S3. MS-curves of CO2 (m/z = 44) of CD powder, PES and PES+CD nanofibers before and after E2 static adsorption (PES+CD PES+CD+E2 Nanofiber).

Supporting information 5: Comparison of IR bands for chlorpyrifos (CP) and polyethersulfone (PES)

Table S3. Comparison of IR bands for CP found in the literature and in the measured samples.

Band	**Measured sample wavenumber (cm^{-1})**	**Literature value (cm^{-1})**	**Ref.**
C=N stretching	1548	1549	17-18
Pyridine stretching	1411	1412	
Ring vibration	1339	1339	
Ring breathing	1164	1165	
C-Cl stretching	1088	1088	
Trigonal ring breathing	1022	1025	
P=S stretching	964	968	

Table S4. Comparison of IR bands for polyethersulfone (PES) found in the literature and in the measured samples.

Band	**Measured sample wavenumber (cm^{-1})**	**Literature value (cm^{-1})**	**Ref.**
Aromatic ether -C_6H_4-O-C_6H_4-	1239	1245	19
Asymmetric O=S=O stretching	1322, 1298	1325 (3 bands: 1324, 1299, and 1289 (shoulder))	
Symmetric O=S=O stretching	1150	1152	
Aromatic ring	1578, 1485	1585, weak 1605, 1488, 1169	

Supporting information 6: IR spectrum of chlorpyrifos (CP)

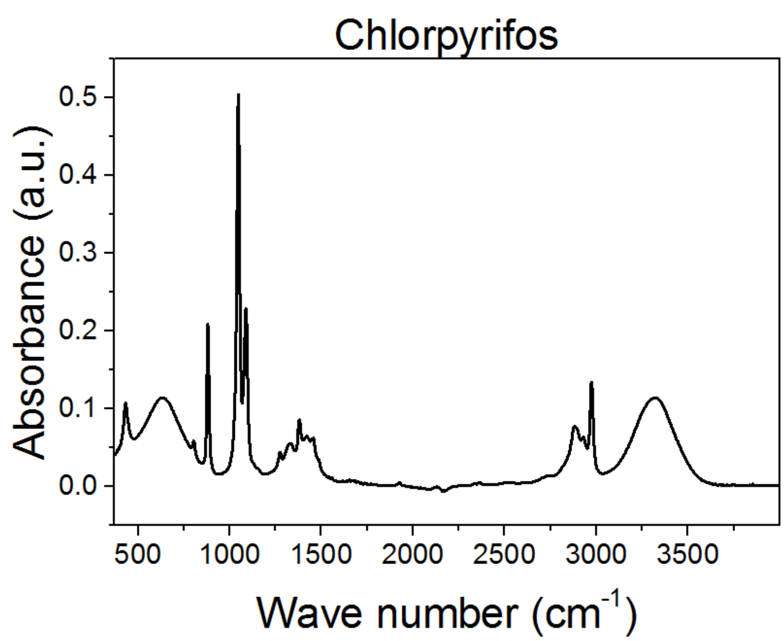

Figure S4. IR spectrum of chlorpyrifos (CP).

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