Supplementary Information

A Critical Review on PFAS in Lithium-Ion Batteries: Application, Monitoring, Exposure and Health Risk

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Table S1 The toxicity-relevant physical-chemical properties of LiB-derived PFAS.

Compound Classification	Compound Name	Molecular Weight	Water Solubility / Hydrophobicity	KOW coefficient	GHS Hazard pictograms	LC50/ LD50/EC50 value
LiB-derived fluoropolymers	PVDF-HFP	$M_n \approx 1.20\times10^5$ $M_w \approx 4.00\times10^5$ [1]	sparingly soluble in water [2]	N A	Non-hazardous[3]	N A
	PVDF-TrFE	M_n=4.9×10^5-2.37×10^6 [4]	insoluble in water [5, 6]	N A	Non-hazardous[3]	N A
	PVDF-CTFE	404,000 [7]	sparingly soluble in water [8, 9]	N A	N A	N A
	PVDF	M_w≈180,000 [10]	insoluble in water [10]	N A	Non-hazardous[3]	N A
	PTFE	M_n= 1.13×10^7-1.19×10^8 [11]	N A	N A	Non-hazardous[3]	LC50: ≈ 2.9 mg/L [12]
	FEP	$M_n \approx 1.25\times10^5$-3.00×10^5 [13]	nearly insoluble in water/dispersible [13, 14]	-1.38 [15]	GHS05 GHS07 [15]	LD50: Rat: 3,300 mg/kg, Rabbit: > 5,000 mg/kg Pimephales promelas (fathead minnow): 39 mg/L; EC50: Daphnia magna (Water flea): 81.2 mg/L [14]
	Fluorinated Polyimide	M_w=9.2×10^4 -15.2×10^4 [16, 17]	insoluble in water [16, 17]	N A	N A	N A
Electrolyte salts	LiTf	156.01 [3, 18]	Soluble in water [3, 18]	N A	GHS07 [3, 18]	N A
	LiTFSI	287.09 [3]	soluble in water [3]	-1.19 [3]	GHS05 GHSO6 GHS08 [3]	LD50: Oral-Rat-female: 210 mg/kg, Dermal-Rabbit:400 mg/kg [3]
	LiFTFSI	237.07 [3]	N A	N A	N A	N A
	LiFSI	187.07 [3]	soluble in water ca.587 g/L at 20 °C [3]	N A	GHS05 GHSO6 GHS08 [3]	LD50：Oral-Rat-female: 300-2,000 mg/kg, Dermal-Rat-female: 2,000-5,000 mg/kg； LC50: Danio rerio (zebra fish): > 74.75mg/L; EC50:Daphnia magna (Water flea):> 100 mg/L [3]
	LiBETI	388.11 [3]	soluble in water [3]	N A	GHS05 GHSO6 [3]	N A

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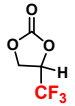
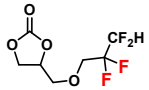
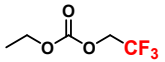
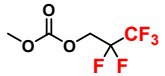
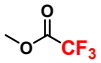
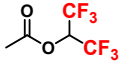
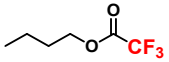
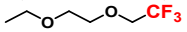
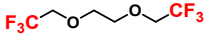
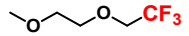
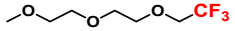
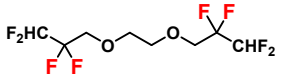
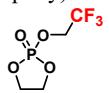
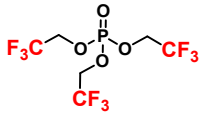
Electrolyte (co-)solvents	BiS-FEtSI	687.14	N A	N A	N A	N A
	LiFNFSI	387.10	N A	N A	N A	N A
	LiTFA	119.96 [3]	N A	N A	GHS07[3]	N A
	LiTDI	192.03 [3]	soluble in water [3]	N A	GHS05 GHSO6 GHS08 [3]	LC50: (Danio rerio; Fundulus heteroclitus; Pimephales promelas): 71.1 mg/L LD50: Oral - Rat female: 300 mg/kg, EC50: Daphnia magna (Water flea): 54 mg/L [3]
	 4,4-difluoro-1,3-dioxolan-2-one (CAS 304881-43-4)	124.04	N A	N A	N A	N A
	 4,4,5-trifluoro-1,3-dioxolan-2-one (CAS 857463-44-6)	142.03	N A	N A	N A	N A
	 3,3,3-trifluoropropylene carbonate (CAS 167951-80-6)	156.06 [19]	N A	0.300 [19]	GHS07 [19]	N A
	 3-(2,2,3,3-tetrafluoropropoxy)propyl-1-ene carbonate (CAS 879496-46-5)	232.13	N A	N A	N A	N A

Compound Classification	Compound Name	Molecular Weight	Water Solubility / Hydrophobicity	KOW coefficient	GHS Hazard pictograms	LC50/ LD50/EC50 value
	 ethyl(2,2,2-trifluoroethyl) carbonate (CAS 156783-96-9)	172.1 [19]	soluble in water [19]	1.6 [19]	GHS02 GHS07 [19]	N A
	 methyl (2,2,3,3,3-pentafluoropropyl) carbonate (CAS 156783-97-0)	208.08	N A	N A	N A	N A
	 methyl trifluoroacetate (CAS 431-47-0)	128.05 [19]	N A	0.600 [19]	GHS02 GHS05 GHS07 [19]	N A
	 methyl 2,2,3,3,4,4,4-heptafluorobutanoate (CAS 356-24-1)	228.06	Slightly soluble in water [19]	2.600 [19]	GHS07 [19]	N A
	 hexafluoroisopropyl acetate (CAS 6919-79-5)	210.07	N A	N A	N A	N A
	 ethyl pentafluoropropionate (CAS 426-65-3)	192.08 [19]	N A	2.100 [19]	GHS02 GHS07 [19]	N A
	 ethyl 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoate (CAS 3108-24-5)	442.12 [20]	N A	5.500 [20]	GHS05 GHS07 GHS08 GHS09 [20]	N A

Compound Classification	Compound Name	Molecular Weight	Water Solubility / Hydrophobicity	KOW coefficient	GHS Hazard pictograms	LC50/ LD50/EC50 value
	 n-butyl trifluoroacetate (CAS 367-64-6)	170.13 [18]	N A	N A	GHS02 GHS05 [18]	N A
	 2-(2-ethoxyethoxy)-1,1,1-trifluoroethane (CAS 260799-56-2)	172.15 [21]	N A	N A	GHS02 GHS05 GHS07 [21]	N A
	 1,2-bis(2,2,2-trifluoroethoxy)ethane (CAS 80054-75-7)	226.12 [22]	N A	2.1442 [22]	GHS07 [22]	N A
	 1,1,1-trifluoro-2-(2-methoxyethoxy)ethane	158.12	N A	N A	N A	N A
	 1,1,1-trifluoro-2-(2-(2-methoxyethoxy)ethoxy) ethane	202.17	N A	N A	N A	N A
	 1,2-bis(2,2,3,3-tetrafluoro propoxy)ethane	290.15	N A	N A	N A	N A
	 3-(2,2,2-trifluoroethoxy)-1,3,2-dioxaphospholane 2-oxide (CAS 67605-68-9)	206.06	N A	N A	N A	N A
	 tris(2,2,2-trifluoroethyl)phosphate (CAS 358-63-4)	344.07 [23]	N A	2.900 [23]	GHS02 GHS07 [23]	N A

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	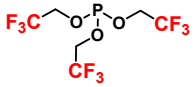 tris(2,2,2-trifluoroethyl) Phosphite (CAS 370-69-4)	328.07 [19]	N A	3.400 [19]	GHS07 [19]	N A
NTf2	NTf2	281.15 [3]	800 g/L (20 °C) [3]	-0.77 (25.5 °C) [3]	GHS05 GHSO6 [3]	LD50: Oral-Rat:50-200 mg/kg, EC50: Daphnia magna (Water flea): 100 mg/l- EC50: Pseudokirchneriella subcapitata (gree n algae):> 100 mg/L [3]
PFOA	Perfluorooctanoic acid	414.07 [24, 25]	highly soluble in water. [26] 9.5 g/L at 25 °C [24]	4.81 [27]	GHS02 GHS05 GHS06 GHS07 GHS08 [3]	LD50: Oral-Rat: 200 - 2000 mg/kg, LC50: Lepomis macrochirus (Bluegill): 15,400.0 mg/L, EC50: Daphnia magna (Water flea): 18,260 mg/L [3, 18]
PFOS	Perfluorooctanesulfonic acid	500.13 [24]	680 mg/L at 25 °C [24]	4.49 [27]	GHS02 GHS06 GHS07 GHS08 GHS09 [3]	LD50: Oral-Rat:154 mg/kg, LC50: Lepomis macrochirus (Bluegill): 15,400.0 mg/L, EC50:Daphnia magna (Water flea): 18,260 mg/L [3, 18]

Table S2 Global distribution of emerging LiB-derived PFAS

Sampling Sites	Sampling Time	Sample Size (n)	Sample Type	LiB-derived PFAS Quantity	Distance	Reference
Guangdong (E-waste recycling park)	2021.01 - 2021.05	109	dust	Bis-FMeSI (NTf2) 123 ng g^{-1}	e-waste sites: two major e-waste recycling facilities; surrounding regions: ranging from 20 to 50 km away; megacity: city of Guangzhou, which is located >100 km from the e-waste sites	[28]
Lithium-Ion Power Battery (LIPB) recycling park	2022.09 - 2023.09	24 environmental sample	18 topsoil,		nine different areas of the site	[29]
			3 dust,	Σ_{16}PFAS 20.78 ng g^{-1}		
			3 sediment	Σ_{16}PFAS 9.88 ng g^{-1}, $TfNH_2$ 2.19 ng g^{-1}		
			3 water	Σ_{16}PFAS 3969.29 g L^{-1}		
		1	LIPB crushing powder			
		2 control samples	1 soil	Σ_{16}PFAS 151.3 ng g^{-1}, $TfNH_2$ 4.43 ng g^{-1}	natural park 4 km away from the LIPB recycling area in the upwind position	
			1 surface water			
USA: Minnesota (3M)/	Minnesota/ Kentucky: 2022.01 - 2022.09 Europe: 2022.10	119 environmental samples	75 surface water, 5 tap water, 2 groundwater, 1 snow, 15 sediment, 21 soil samples	soil : Bis-FMeSI 2300 ng kg^{-1}	USA: Closest: 0 km (direct discharge); farthest: 21 km (MN27, Minnesota)	[30]
				surface water: Bis-FMeSI 440-2437 ng L^{-1}		
				snow: Bis-FMeSI 6.88 ng L^{-1}		
				sediment: Bis-FMeSI 1626 ng Kg^{-1}		
Kentucky (Arkema);				surface water: Bis-FMeSI 2.69 ng L^{-1}, PFDA 1.25 ng L^{-1}, PFOS 19.7ng L^{-1}		
Europe: Antwerp (3M)/				surface water: Bis-FMeSI 81.9 ng L^{-1}, Bis-FEtSI 65.7 ng L^{-1}		
				sediment : Σ3Bis-PASI 10746 ng kg^{-1}		
				soil: Σ3Bis-PASI 650 ng kg^{-1}		
Salindres (Solvay)				surface water: Bis-FMeSI 6.55 ng L^{-1}		
				sediment: ΣBis-PASI 3886 ng kg^{-1}		
				soil: ΣBis-PASI 253 ng kg^{-1}		
		17 product samples	batteries			
		2 waste samples	leachates collected from different			

			municipal landfills			
		1 materials samples	PVDF battery binder			
region A (Fujian);	A: 2023.08	74	12 water	N-MeFMeSA 129 ng L^{-1} N-EtFMeSA 41 ng L^{-1} N-MeFMeSH 597 ng L^{-1}	surrounding areas receiving runoff or outfall discharges	[31]
			12 sediment			
region B (Shandong);	B: 2023.08		11 water	Di-FMeS 32-253 ng L^{-1} PFPrDiSI 7.8-55 ng L^{-1}		
			11 sediment	Di-FMeS 3.0-61 ng g^{-1} PFPrDiSI 10-110 ng g^{-1}		
region C Jiangsu)	C: 2023.07		14 water			
			14 sediment	NMeFMeSA 1.4-34 ng g^{-1} N-EtFMeSA 7.3-54 ng g^{-1}		
	2023.07 - 2023.08	6-10 control samples	water, sediment		control: rivers or lakes located 20–40 km away from the sampling region	
Taihu Lake	2021.10 - 2022.07	192	96 water, 96 sediment	Bis-FMeSI 21.7 ng L^{-1}	Not reported	[32]
Australia	Not reported	63	3 ground water,	PFPrA 567 ng L^{-1} PFEtS 162 ng L^{-1} PFPrS 8100 ng L^{-1}	Not reported	[33]
			33 surface water,	PFEtS 0.76 ng L^{-1} PFPrS 68 ng L^{-1}		
			6 waste water,			
			21 drinking water	PFPrS 0.02 ng L^{-1}		
Germany	2020.10.27 - 2020.11.4	46	16 surface water,	TFA 12.4 μg L^{-1} NTf2 2.0 ng L^{-1}	Not reported	[34]
			16 bank filtrate,			
			7 raw water,			
			7 groundwater			
Shanghai	Shanghai: 2021.07	45	39 tapwater: (Shanghai)	TFMS, NTf2	Not reported	[35]
	Sweden, Denmark, and Norway: 2022		6 tap water: (Sweden, Denmark, and Norway)			

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