Electronic Supporting information

Assessment of the environmental and human health impact in the synthesis and processing of metal halide perovskite active layers using GVL

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1. Experimental methods

1.1 Goal and scope definition

The primary objective of the LCA study presented is to evaluate the environmental sustainability of manufacturing a metal-halide perovskite (MHP) active layer ($MAPbI_3$ and $FAPbI_3$) using GVL as a green reaction and processing solvent, and to compare its impact with that of GBL and DMF.

The experimental procedures referenced in this study for the impact evaluation of $MAPbI_3$ and $FAPbI_3$ production using GVL, GBL, and DMF as solvents (or solvent mixture in the case of $FAPbI_3$, where they are the predominant portion) were sourced from existing literature (secondary data).[1-4]

The functional unit was defined as 1 g of the desired target product. At the same time, the system boundary was determined based on a cradle-to-gate approach, considering the emissions and resource exploitation for both the extraction and manufacturing of all materials and energy, as well as the respective processes' emissions to water, air, and soil. Moreover, it was assumed that all the processes analyzed were performed at one location and that the synthesis proposals were set only to produce the active layer without by-products. The environmental effects of transporting raw materials have been included (100 km by lorry > 16 t and 600 km by train), as well as the impact of chemical factories, i.e. the infrastructures and facilities considered for the manufacturing processes. (4.00E-13 unit).

1.2 Inventory analysis

While setting up the LCA analysis, new inventories for different materials have been created to be included in the model, adopting a retrosynthetic approach. If an existing inventory data set was available for a specific compound that needed to be modelled, it was considered and utilized in the study.

General assumptions were made regarding process energy (0.0002 MJ per gram of the compound) and electricity consumption (0.000333 kWh per gram of the compound) for all unavailable compounds that required specific modeling.[5]

Considering the European Union's statements, the contribution of electricity in the final synthetic steps for producing the perovskite active layer (i.e., active layer synthesis and processing) has been excluded from the analysis, as it is nearly identical across all the procedures studied. Instead, the focus has been placed on the impact of the chemicals used, specifically the environmental and human health effects associated with the choice of one solvent over another.

The emissions to air during the synthetic processes (0.20% volatile input materials) and air (CO_2), as well as water (river) and sludge emissions after wastewater treatment, were calculated. No emissions to the soil were determined, as no agricultural destination for the digested sludge was considered. In this wastewater treatment, 65.80% of the organic compounds were retained in the sludge, 24.50% were oxidized and released into the air as CO_2, and the remaining 9.70% were discharged into the river.[5]

Assumptions regarding data gaps (e.g., solvent amount) were made based on our expertise and are clearly outlined in the corresponding inventory tables.

For inventories already available in the literature, material flows were adopted and adjustments were made to reflect our approach to electricity and steam consumption.

1.3 Impact assessment

The impact assessment was performed using SimaPro 9.6 software and the ReCiPe 2016 method, considering 18 impact categories (*Global warming, Stratospheric ozone depletion, Ionizing radiation, Ozone formation, Human health, Fine particulate matter formation, Ozone formation, Terrestrial ecosystems, Terrestrial acidification, Freshwater eutrophication, Marine eutrophication, Terrestrial ecotoxicity, Freshwater ecotoxicity, Marine ecotoxicity, Human carcinogenic toxicity, Human non-carcinogenic toxicity, Land use, Mineral resource scarcity, Fossil resource scarcity, Water consumption*).[6]

Midpoint impact categories and endpoint damage areas (*Human health*, *Ecosystems*, and *Resources*) were analyzed from a hierarchical perspective over a 100-year period. Long-term emissions, which affect scenarios beyond 100 years, were excluded due to their high uncertainties and their relationship to heavy metal toxicity. Therefore, they are not particularly relevant in organic chemical processing. The results from the various protocols examined are presented and analyzed in midpoints, with outcomes weighted and normalized in endpoint damage areas. This enables a comparison of our approach with others using a single indicator as a benchmark for global environmental impact. During this process, midpoint characterization results are transformed into intermediate units, which are then weighted and normalized to represent the relative impact in micropoints (μPts), reflecting their severity within a global context.

2. Characterization

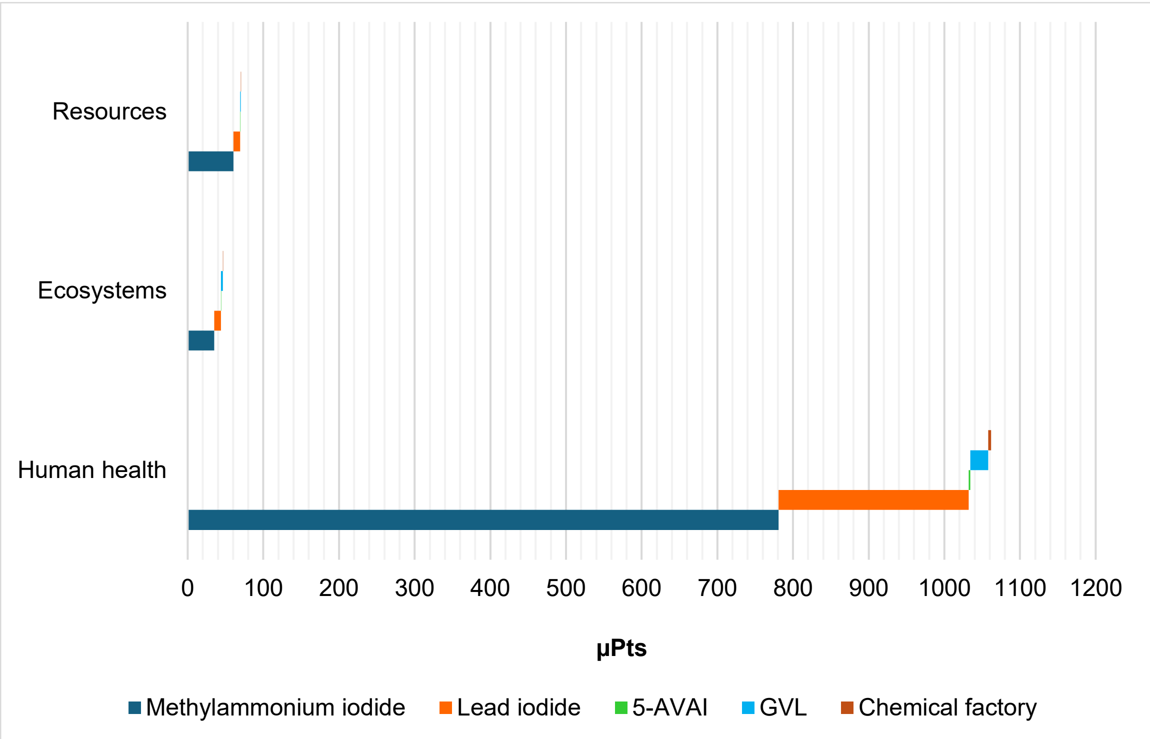

Figure ESI-1. Endpoint single score contribution in the damage areas for the $MAPbI_3$ manufacturing process in GVL.

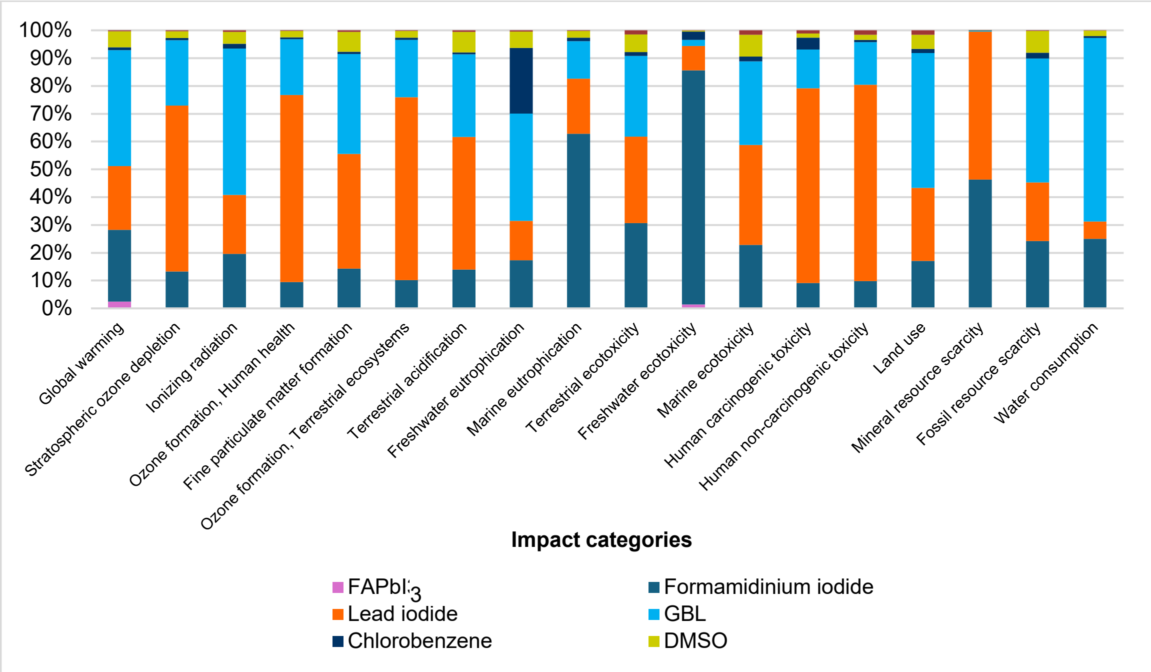

Figure ESI-2. Midpoint characterization deriving from the manufacturing of $FAPbI_3$ in GBL:DMSO (7:3)

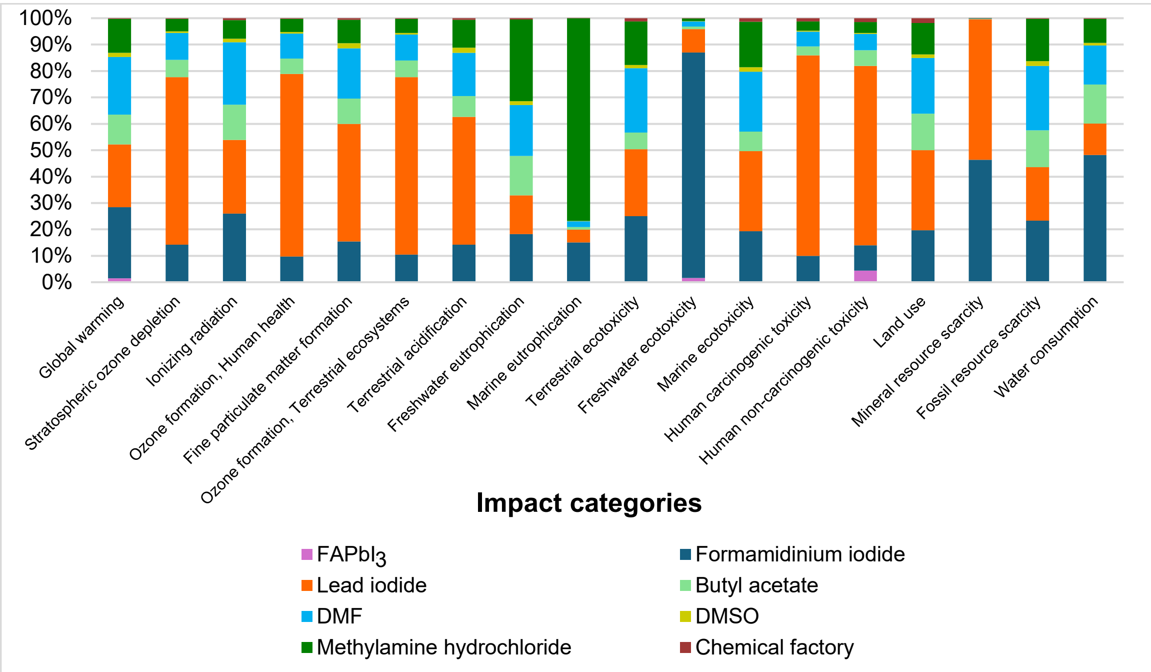

Figure ESI-3. Midpoint characterization deriving from the manufacturing of $FAPbI_3$ in DMF:DMSO (9:1)

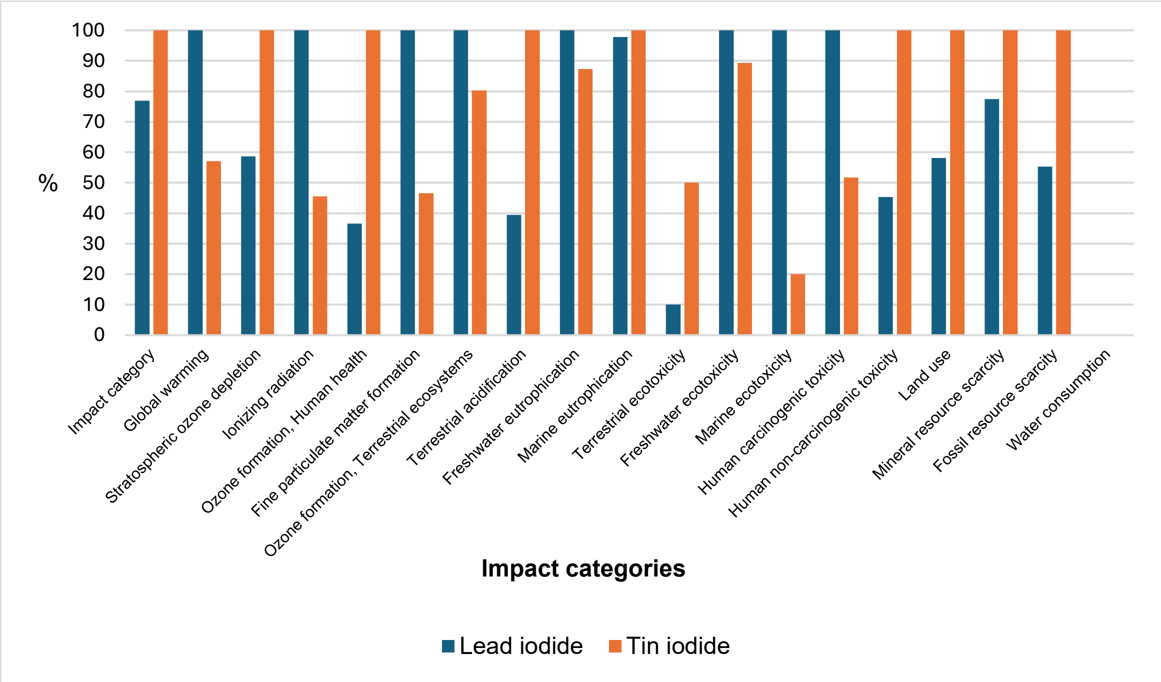

Figure ESI-4. Midpoint analysis comparison between lead iodide and tin iodide

2. LCA Inventore dataset

2.1 Inventories for the reference processes

Table ESI-1. Synthesis of $MAPbI_3$ in GVL[1]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Methylammonium iodide	0.2534057	-	-	-	-
Lead iodide	0.734874	-	-	-	-
5-ammonium valeric acid iodide	0.011719	-	-	-	-
γ-Valerolactone	1.386825	0.002277	0.339770	0.134522	0.91253
Chemical factory	4xE-13 p	-	-	-	-

Table ESI-2. Synthesis of $MAPbI_3$ in GBL[1]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Methylammonium iodide	0.2534057	-	-	-	-
Lead iodide	0.734874	-	-	-	-
5-ammonium valeric acid iodide	0.011719	-	-	-	-
γ-butyrolactone	1.178946	0.002360	0.288884	0.114357	0.775746
Chemical factory	4xE-13 p	-	-	-	-

Table ESI-3. Synthesis of $MAPbI_3$ in DMF[2]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Methylammonium iodide	0.2534057	-	-	-	-
Lead iodide	0.734874	-	-	-	-
5-ammonium valeric acid iodide	0.011719	-	-	-	-
N,N-Dimethylformamide	1.354307	0.002709	0.331805	0.131367	0.891134
Chemical factory	4xE-13 p	-	-	-	-

Table ESI-4. Synthesis of $FAPbI_3$ in GVL[3]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Formamidinium iodide	0.271683	-	-	-	-
Lead iodide	0.728316	-	-	-	-
butyl acetate	0.410058	0.000820116	0.100263282	0.039696075	0.269278528
Methylamine hydrochloride	0.037334	-	-	-	-
γ-Valerolactone	0.975776	0.001951552	0.23858699	0.094460971	0.640776487
Chemical factory	4xE-13 p	-	-	-	-

Table ESI-5. Synthesis of $FAPbI_3$ in GBL:DMSO (7:3)[4]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Formamidinium iodide	0.27175	-	-	-	-
Lead iodide	0.72995	-	-	-	-
γ-Butyrolactone	1.249763	1.249763	0.002499526	0.305579551	0.120984557
Dimethylsulfoxide	0.412374	0.412374	0.000824748	0.100829567	0.039920277
Chlorobenzene	0.087372	0.087372	0.000174744	0.021363328	0.008458134
Chemical factory	4xE-13 p	-	-	-	-

Table ESI-6. Synthesis of $FAPbI_3$ in DMF:DMSO (9:1)[3]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Formamidinium iodide	0.271683	-	-	-	-
Lead iodide	0.728316	-	-	-	-
Butyl acetate	0.410058	0.000820116	0.100263282	0.039696075	0.269278528
Methylamine hydrochloride	0.037334	-	-	-	-
N,N-dimethylformamide	0.786197	0.001572394	0.192233028	0.076108587	0.516282991
Dimethylsulfoxide	0.102224	0.000204448	0.02499479	0.009895897	0.067128865
Chemical factory	4xE-13 p	-	-	-	-

2.2 Inventories for the needed compounds in the synthesis approaches that were not available in life cycle databases.

Table ESI-7. Synthesis of 5-ammonium valeric acid iodide (5-AVAI)[7]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
formic acid	-	-	-	-	-
1,4-butanediol	-	-	-	-	-
ammonia, liquid	-	-	-	-	-
Hydrogen, gasseous	-	-	-	0.146996[a]	-
Iiodine	-	-	-	-	-
Transport, lorry 16-32	1xE-4 tkm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ				
Electricity	0.000333 KWh	-	-	-	-

[a]as H_2O

Table ESI-8. Synthesis of lead iodide (PbI_2)[8]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Iodine	0.67	0.00134	-	-	-
Potassium hydroxide	0.291	-	-	0.438[b]	-
Lead	0.449		-	-	-
Nitric acid	0.729	0.00146	0.0434[a]		-
Transport, lorry 16-32	1xE-4 tkm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ				
Electricity	0.000333 KWh	-	-	-	-

[a]as nitrogen monoxide; [b]as potassium nitrate

Table ESI-9. Synthesis of Methylammonium iodide (MAI)[9]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Iodine	1.4	-	-	-	-
Hydrogen sulfide	0.14	0.120[a]	-	-	-
Methylamine	0.58	-	-	-	-
Ethanol abs.	7.3	-	-	-	-
Diethyl ether	20.8	-	-	-	-
treatment of spent solvent mixture, hazardous waste incineration					29.9[b]
Transport, lorry 16-32	1xE-4 tkm	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ				
Electricity	0.000333 KWh	-	-	-	-

[a]as Solfur; [b]Hazardous waste incineration

Table ESI-10. Synthesis of γ-valerolactone (GVL)[10]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)			Waste treatment (g)
			CO_2 to air	Compounds to river	Final waste flow (sludge)	
Stalk	4.601	-	-	-	-	0.367
Sulfuric acid	0.046	-	-	-	-	
Lime (calcium hydroxide)	0.035	-	-	-	-	
Water	1.872	-	-	-	-	
Hydrogen, gasseous	0.016	-	-	-	-	
Transport, lorry 16-32	1xE-4 tkm	-	-	-	-	
Transport train	6.00E-04 tkm	-	-	-	-	
Chemical factory	4xE-13 p	-	-	-	-	
Steam	0.0002 MJ	-	-	-	-	

Electricity	0.000333 KWh	-	-	-	-	

Table ESI-11. Synthesis of hydriodic acid (HI)[11]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Iodine	0.9921270				
Idrazine	0.0626310		0.0547251[a]		
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]As nitrogen

Table ESI-12. Synthesis of formamidine acetate (FAAc)[12]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Acetic acid	0.885	solvent spent mixture = 1.43g			
Ammonia	0.365				
Hydrochloric acid	0.417				
Hydrogen cyanide	0.281				
Nitrogen gaseous	0.288				
Ethanol	0.479				
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

Table ESI-13. Synthesis of formamidinium iodide (FAI)[12]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)[a]		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
formamidine acetate	0.657	-	-	-	-
Solvent	4.5	-	-	-	-
Hydriodic acid	1.62	-	0.00162[b]	-	-

Nitrogen, gaseous	0.288	-	-	-	-
Cooling water	400	-	-	-	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]output waste treated as "spent solvent mixture" (1.90 g); [b]As hydriodic acid

Table ESI-14. Synthesis of methylamine hydrochloride (MACl)[13]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Hydrochloric acid	0.543031	0.001086	-	-	-
Methylamine	0.552739	0.001105	0.022370705	0.008856973	0.060081322
H_2O	1.102517	0.002205	-	1.100311966	-
Ethanol	1.675004	0.00335	0.41037598	0.162475388	1.102152632
Acetonitrile	10[a]	0.02	2.45	0.97	6.58
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	-	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]Assumed because not specified

Table ESI-15. Synthesis of tin chloride ($SnCl_2$)[12]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Hydrochloric acid	0.414	-	0.000414[a]	-	-
Nitrogen, gasseous	0.288	-	-	-	-
Tin	0.684	-	-	-	-
H_2O	-	-	-	4.60	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	0.0153 MJ	-	-
Electricity	0.000333 KWh	-	-	-	-

[a]As hydrochloric acid

Table ESI-16. Synthesis of tin iodide (SnI_2)[12]

Inputs	Quantity (g) for 1 g of product	Process air emissions (g)	Wastewater treatment emissions (g)		
			CO_2 to air	Compounds to river	Final waste flow (sludge)
Tin chloride	0.551	-	-	-	-
Iodine	0.74	-	-	-	-
Nitrogen, gasseous	0.288	-	-	-	-
H_2O	-	-	-	4.79	-
Transport train	6.00E-04 tkm	-	-	-	-
Chemical factory	4xE-13 p	-	-	-	-
Steam	0.0002 MJ	-	0.0153 MJ	-	-
Electricity	0.000333 KWh	-	-	-	-

3. LCA impact assessment dataset

Table ESI-17. Midpoint characterization (%) of the chemicals used in the manufacturing process of $MAPbI_3$ in GVL

Impact category	Total (%)	MAI	PbI_2	5-AVAI	GVL	Chemical factory
Global warming	100	83,009572	13,704503	0,199155	2,002760	0,169522
Stratospheric ozone depletion	100	39,739084	38,763122	0,118453	21,195998	0,183342
Ionizing radiation	100	74,650190	17,488782	0,309055	7,128498	0,423476
Ozone formation, Human health	100	52,333709	45,654168	0,098659	1,761272	0,152193
Fine particulate matter formation	100	61,990163	33,386541	0,198896	3,923008	0,501392
Ozone formation, Terrestrial ecosystems	100	57,247385	40,877556	0,093773	1,642290	0,138996
Terrestrial acidification	100	58,286034	35,520762	0,168340	5,583842	0,441023
Freshwater eutrophication	100	94,571696	2,374938	0,030359	2,950379	0,072628
Marine eutrophication	100	36,414783	6,663185	0,060081	56,787993	0,073957
Terrestrial ecotoxicity	100	78,856008	16,715263	0,143391	3,469823	0,815515
Freshwater ecotoxicity	100	50,391702	44,943008	0,082995	4,042730	0,539565
Marine ecotoxicity	100	78,727002	16,838958	0,122714	3,541903	0,769423
Human carcinogenic toxicity	100	43,842770	53,087453	0,086977	2,141459	0,841341
Human non-carcinogenic toxicity	100	59,757946	58,202196	0,101077	-19,332204	1,270984
Land use	100	54,313440	8,884422	0,105943	36,157383	0,538813

Mineral resource scarcity	100	42,001263	57,171850	0,687551	0,097533	0,041802
Fossil resource scarcity	100	92,154978	6,668653	0,110588	0,996219	0,069561

Table ESI-18. Midpoint characterization (%) of the chemicals used in the manufacturing process of $MAPbI_3$ in GBL

Impact category	Total (%)	MAI	PbI_2	5-AVAI	GBL	Chemical factory
Global warming	100	68,50573	11,30998	0,164358	19,23835	0,139902
Stratospheric ozone depletion	100	42,67338	41,62535	0,1272	15,37719	0,19688
Ionizing radiation	100	55,84787	13,08384	0,231212	30,52026	0,316814
Ozone formation, Human health	100	47,15552	41,13689	0,088897	11,48155	0,137134
Fine particulate matter formation	100	50,24113	27,05877	0,161199	22,13254	0,406363
Ozone formation, Terrestrial ecosystems	100	51,85367	37,02617	0,084938	10,90933	0,1259
Terrestrial acidification	100	50,63734	30,85949	0,146249	17,97377	0,383149
Freshwater eutrophication	100	91,68306	2,302397	0,029432	5,914698	0,070409
Marine eutrophication	100	76,74831	14,04342	0,126628	8,925762	0,155874
Terrestrial ecotoxicity	100	70,9395	15,03718	0,128996	13,16068	0,733644
Freshwater ecotoxicity	100	47,33139	42,21359	0,077955	9,870266	0,506797
Marine ecotoxicity	100	71,77029	15,35098	0,11187	12,06542	0,701433
Human carcinogenic toxicity	100	40,67318	49,24952	0,080689	9,216091	0,780517
Human non-carcinogenic toxicity	100	45,58101	44,39434	0,077098	8,978097	0,969457
Land use	100	68,5946	11,22049	0,133799	19,37062	0,680488
Mineral resource scarcity	100	41,91409	57,05319	0,686124	0,304889	0,041716
Fossil resource scarcity	100	82,14963	5,944632	0,098582	11,74515	0,062009

Table ESI-19. Midpoint characterization (%) of the chemicals used in the manufacturing process of $MAPbI_3$ in DMF

Impact category	Total (%)	MAI	PbI_2	5-AVAI	DMF	Chemical factory
Global warming	100	69,48548	11,47174	0,166708	17,98661	0,141903
Stratospheric ozone depletion	100	44,49522	43,40245	0,13263	11,76442	0,205286
Ionizing radiation	100	63,23939	14,8155	0,261814	21,32455	0,358744

Ozone formation, Human health	100	48,03304	41,90241	0,090551	9,834315	0,139686
Fine particulate matter formation	100	51,45671	27,71345	0,165099	20,24855	0,416195
Ozone formation, Terrestrial ecosystems	100	52,73796	37,6576	0,086386	9,390007	0,128047
Terrestrial acidification	100	50,72071	30,91029	0,14649	17,83873	0,38378
Freshwater eutrophication	100	92,39802	2,320352	0,029662	5,181008	0,070958
Marine eutrophication	100	75,17984	13,75643	0,12404	10,787	0,152688
Terrestrial ecotoxicity	100	63,62298	13,48629	0,115692	22,11541	0,657978
Freshwater ecotoxicity	100	44,26942	39,48271	0,072912	14,26631	0,474011
Marine ecotoxicity	100	66,72524	14,2719	0,104006	18,24308	0,652126
Human carcinogenic toxicity	100	41,97023	50,82006	0,083262	6,321042	0,805407
Human non-carcinogenic toxicity	100	44,31171	43,15809	0,074951	6,669396	0,94246
Land use	100	73,04438	11,94837	0,142479	14,14014	0,724632
Mineral resource scarcity	100	41,93666	57,08391	0,686494	0,251194	0,041738
Fossil resource scarcity	100	81,76445	5,916759	0,098119	12,15895	0,061718

Table ESI-20. Midpoint characterization (%) of the chemicals used in the manufacturing process of $FAPbI_3$ in GVL

Impact category	Total (%)	$FAPbI_3$	FAI	PbI_2	Butyl acetate	MACl	GVL	Chemical factory
Global warming	100	2.016474	34.012437	30.030493	14.225031	16.225093	3.115657	0.374815
Stratospheric ozone depletion	100	0.000000	12.434444	55.765300	5.786060	4.099918	21.648144	0.266134
Ionizing radiation	100	0.000000	31.234388	33.606101	16.131991	8.481709	9.724741	0.821070
Ozone formation, Human health	100	0.100244	10.567635	75.251951	6.373500	5.392516	2.061035	0.253119
Fine particulate matter formation	100	0.000000	18.716202	53.735829	11.631777	10.619299	4.482633	0.814260
Ozone formation, Terrestrial ecosystems	100	0.156674	11.217109	73.583814	6.834548	5.856606	2.098789	0.252459
Terrestrial acidification	100	0.000000	16.258346	55.551558	9.120836	12.173656	6.199670	0.695934
Freshwater eutrophication	100	0.000000	19.727766	16.009220	16.111068	33.538535	14.119428	0.493983
Marine eutrophication	100	0.000000	11.944303	3.771601	0.806590	60.614938	22.820328	0.042240
Terrestrial ecotoxicity	100	0.008503	32.044186	32.512366	7.966193	21.076816	4.791419	1.600517
Freshwater ecotoxicity	100	1.429013	86.816882	8.975729	1.044668	1.051782	0.573197	0.108729

Marine ecotoxicity	100	0.069821	23.993715	37.893460	9.164966	21.472403	5.658577	1.747058
Human carcinogenic toxicity	100	0.000000	10.359192	78.919392	3.563535	3.635812	2.260076	1.261993
Human non-carcinogenic toxicity	100	0.000000	13.025829	93.113007	8.227116	5.539436	-21.957043	2.051654
Land use	100	0.000000	11.894773	18.357966	8.431096	7.151524	53.041262	1.123379
Mineral resource scarcity	100	0.000000	46.462473	53.244883	0.086873	0.102002	0.064487	0.039282
Fossil resource scarcity	100	0.000000	30.777047	26.709542	18.254446	21.145120	2.832726	0.281119

Table ESI-21. Midpoint characterization (%) of the chemicals used in the manufacturing process of $FAPbI_3$ in GBL:DMSO (7:3)

Impact category	Total (%)	$FAPbI_3$	FAI	PbI_2	GBL	Chlorobenzene	DMSO	Chemical factory
Global warming	100	2.392606	25.904058	22.917048	41.602369	1.085066	5.813462	0.285391
Stratospheric ozone depletion	100	0.000000	13.273345	59.646399	23.515632	0.756497	2.524108	0.284019
Ionizing radiation	100	0.000000	19.634256	21.167313	52.695330	1.633265	4.353831	0.516006
Ozone formation, Human health	100	0.089362	9.422704	67.232874	20.026467	0.663821	2.339133	0.225639
Fine particulate matter formation	100	0.000000	14.323590	41.206363	35.970049	0.753384	7.123610	0.623003
Ozone formation, Terrestrial ecosystems	100	0.139664	10.001713	65.741854	20.672100	0.779234	2.440385	0.225049
Terrestrial acidification	100	0.000000	13.939626	47.724038	29.664789	0.763853	7.311160	0.596535
Freshwater eutrophication	100	0.000000	17.329150	14.090801	38.631492	23.636595	5.878146	0.433815
Marine eutrophication	100	0.000000	62.794065	19.867797	13.476452	1.210294	2.429383	0.222009
Terrestrial ecotoxicity	100	0.008223	30.606824	31.116001	29.063578	1.343946	6.333079	1.528348
Freshwater ecotoxicity	100	1.422725	84.243144	8.727027	2.177691	2.937588	0.386346	0.105479
Marine ecotoxicity	100	0.067105	22.710940	35.939170	30.145875	1.672813	7.810849	1.653248
Human carcinogenic toxicity	100	0.000000	9.166232	69.970481	13.973754	4.214532	1.558613	1.116388
Human non-carcinogenic toxicity	100	0.000000	9.856553	70.598622	15.237245	0.844881	1.910609	1.552090
Land use	100	0.000000	17.028333	26.333387	48.516791	1.500668	5.013009	1.607812
Mineral resource scarcity	100	0.000000	46.360859	53.234504	0.303605	0.016862	0.044984	0.039186
Fossil resource scarcity	100	0.000000	24.254564	21.091095	44.471944	2.158724	7.802185	0.221488

Table ESI-22. Midpoint characterization (%) of the chemicals used in the manufacturing process of $FAPbI_3$ in DMF:DMSO (9:1)

Impact category	Total (%)	$FAPbI_3$	FAI	PbI_2	Butyl acetate	DMF	DMSO	MACl	Chemical factory
Global warming	100	1.496770	26.944893	23.790368	11.269170	21.848853	1.499382	12.853633	0.296931
Stratospheric ozone depletion	100	0.000000	14.163540	63.519855	6.590652	10.084936	0.667833	4.670041	0.303142
Ionizing radiation	100	0.000000	25.958271	27.929353	13.406973	23.546795	1.427255	7.048977	0.682375
Ozone formation, Human health	100	0.092023	9.700914	69.080046	5.850768	9.496532	0.597119	4.950240	0.232359
Fine particulate matter formation	100	0.000000	15.490655	44.475005	9.627159	19.033846	1.910235	8.789170	0.673931
Ozone formation, Terrestrial ecosystems	100	0.143308	10.260123	67.306027	6.251460	9.830476	0.620733	5.356951	0.230921
Terrestrial acidification	100	0.000000	14.175492	48.434858	7.952367	16.372918	1.843495	10.614091	0.606778
Freshwater eutrophication	100	0.000000	18.185970	14.758041	14.851930	19.301738	1.529566	30.917378	0.455377
Marine eutrophication	100	0.000000	15.114288	4.772574	1.020657	2.192073	0.144989	76.701971	0.053450
Terrestrial ecotoxicity	100	0.008479	25.018099	25.383625	6.219506	24.381675	1.283570	16.455462	1.249584
Freshwater ecotoxicity	100	1.602921	85.428524	8.832191	1.027962	1.869307	0.097143	1.034962	0.106990
Marine ecotoxicity	100	0.060717	19.231074	30.371784	7.345763	22.740187	1.639968	17.210230	1.400275
Human carcinogenic toxicity	100	0.000000	9.967818	75.937790	3.428903	5.532466	0.420258	3.498449	1.214315
Human non-carcinogenic toxicity	100	4.455561	9.499517	67.905745	5.999897	6.146644	0.456580	4.039817	1.496237
Land use	100	0.000000	19.643716	30.317407	13.923600	21.015723	1.433899	11.810441	1.855213
Mineral resource scarcity	100	0.000000	46.423509	53.200232	0.086800	0.137125	0.011169	0.101917	0.039249
Fossil resource scarcity	100	0.000000	23.356205	20.269441	13.853005	24.398404	1.862918	16.046691	0.213337

Table ESI-23. Endpoint-single score (μPts) details for the three damage areas considered in the synthesis $MAPbI_3$

Procedure	Total	Human health	Ecosystems	Resources
$MAPbI_3$ in GVL	1185	1068	47	70
$MAPbI_3$ in GBL	1441	1311	55	75
$MAPbI_3$ in DMF	1409	1280	53	76

Table ESI-24. Endpoint-single score (µPts) details for the three damage areas considered in the synthesis of $FAPbI_3$

Procedure	Total	Human health	Ecosystems	Resources
$FAPbI_3$ in GVL	611	565	23	23
$FAPbI_3$ in GBL:DMSO (7:3)	798	745	28	25
$FAPbI_3$ in DMF:DMSO (9:1)	749	696	27	27

Table ESI-25. Endpoint-single score (µPts) details for the three damage areas considered in the comparison among PbI_2 and SnI_2

Procedure	Total	Human health	Ecosystems	Resources
PbI_2	366	342	12	12
SnI_2	718	687	12	19

References

1. C. Worsley, D. Raptis, S. Meroni, A. Doolin, R. Garcia-Rodriguez, M. Davies and T. Watson, *Energy Technol.*, 2021, **9**, 1–10.

2. A. Karavioti, E. Vitoratos and E. Stathatos, *J. Mater. Sci. Mater. Electron.*, 2020, **31**, 6109–6117.

3. Y. Miao, M. Ren, Y. Chen, H. Wang, H. Chen, X. Liu, T. Wang and Y. Zhao, *Nat. Sustain.*, 2023, **6**, 1465–1473.

4. Y. Liu, J. Sun, Z. Yang, D. Yang, X. Ren, H. Xu, Z. Yang and S. F. Liu, *Adv. Opt. Mater.*, 2016, **4**, 1829–1837.

5. F. Campana, K. Zhou, J. A. Yunda, A. Nazari, D. Bonifazi, S. Melinte and L. Vaccaro, *Chem. Eng. J.*, 2025, **504**, 158822.

6. M. A. J. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander and R. van Zelm, *Int. J. Life Cycle Assess.*, 2017, **22**, 138–147.

7. J. A. Alberola-Borràs, J. A. Baker, F. De Rossi, R. Vidal, D. Beynon, K. E. A. Hooper, T. M. Watson and I. Mora-Seró, *iScience*, 2018, **9**, 542–551.

8. J. Gong, S. B. Darling and F. You, *Energy Environ. Sci.*, 2015, **8**, 1953–1968.

9. A. Ali Khan, PhD thesis, University of Freiburg, September 2020.

10. J. Han, M. Son and D. Kang, *J. Ind. Eng. Chem.*, 2023, **120**, 254–260.

11. N. N. Greenwood and A. Earnshaw, *The Chemistry of the Elements*, 2nd edn, Butterworth-Heinemann, Oxford, 1997, pp. 809–815.

12. J. Zhang, X. Gao, Y. Deng, Y. Zha and C. Yuan, *Sol. Energy Mater. Sol. Cells*, 2017, **166**, 9–17.

13. Y. Zhao and K. Zhu, J. *Phys. Chem. C,* 2014, **118**, 9412−9418.