Lead-Free Alternatives and Toxicity Mitigation Strategies for Sustainable Perovskite Solar Cells: A Critical Review

Table S1: Toxicity of frequently used additives

Group	Material	Nature of Toxicity	Reference
Carbonyl	polymerizable acrylamide monomer	Neurotoxic, carcinogenic, skin and eye irritant	https://pubchem.ncbi.nlm.nih.gov/compound/6579
	poly (butylene adipate-co-terephthalate) (PBAT) polymer	Although PBAT is not poisonous, its breakdown products, adipic acid and terephthalic acid, can harm the environment and soil microbial populations, impacting ecosystem health.	[1], [2]
	poly (acrylic acid) having a carbonyl group	Generally considered non-toxic	[3]
Porphyrin	polymerized zinc porphyrin (ZnP) additive	Limited Data	-
	fullerene-porphyrin dyad (FPD) having a porphyrin ring as well as pentafluorophenyl groups	Limited data	
	$H_3PMo_{12}O_{40}$ to a zirconium-porphyrin-based MOF-545 (P@Ms)	Limited data	
Thiol	3-mercaptopropyl-tri-ethoxy-silane	Skin and eye irritant; harmful if inhaled or ingested.	https://www.gelest.com/wpcontent/uploads/product_msds/SIM6476.0-msds.pdf
	perfluorocarbon tail-chains of 1H, 1H, 2H, 2H perfluorodecanethiol	Inhalation - May cause respiratory irritation.	https://www.chemicalbook.com/msds/1h-1h-2h-2h-perfluorodecanethiol.htm
	thiol group of 1H, 1H, 2H, 2H perfluorodecanethiol	It may cause skin, eye, and liver irritation. It may also be harmful if swallowed.	https://www.sigmaaldrich.com/MY/en/product/aldrich/660493
sulfonic acid	amphoteric phenylbenzimidazole sulfonic acid	Used in sunscreens; may cause skin irritation in sensitive individuals.	https://procoal.co.uk/blogs/skin-school/phenylbenzimidazole-sulfonic-acid#:~:text=Side%20effects%20of%20Phenylbenzimidazole%20Sulfonic,hours%20to%20avoid%20allergic%20reactions.
	phenylbenzimidazole sulfonic acid	It is a UV-B absorber used in cosmetics and sunscreens. It can cause skin irritation and allergic reactions.	[4]
	cation-exchange resin (CER) having two sulfonate groups	Limited data	
Aniline	ligand molecule 4-[(trifluoromethyl) sulphanyl]-aniline (4TA) with trifluoromethyl ($-CF_3$) and aniline ($-NH_2$) moieties	The trifluoromethyl group's increased lipophilicity and the possible reactivity of the aniline group—which might disturb cellular functions—cause it to be poisonous.	*https://www.sigmaaldrich.com/MY/en/product/aldrich/224936* *.https://pubchem.ncbi.nlm.nih.gov/compound/9964*
Spiro-NPU	1,5-naphthalene diisocyanate (NDI) and (2,20,20,200'-(((9,90-spirobi[fluorene]-2,20,7,70 tetrayltetrakis (phe-nylazanediyl))	Spiro-NPU contains NDI, a respiratory sensitizer and irritant that can cause respiratory difficulties, skin and eye irritation, allergic responses, and long-term damage to aquatic life. Inhalation can be	https://echa.europa.eu/substance-information/-/substanceinfo/100.019.675

	tetrakis (ethane-2,1-diyl))tetrakis(oxy))tetrakis(-etan-1-ol)) (Spiro-OH)	lethal.	
Phosphate Compounds	Na_3PO_4	It can cause kidney damage, skin irritation, and respiratory issues.	https://core-docs.s3.amazonaws.com/documents/asset/uploaded_file/234350/Sodium_Phosphate_Tribasic.pdf https://medlineplus.gov/druginfo/meds/a609019.html#:~:text=Sodium%20phosphate%20can%20cause%20serious,%2C%20decreased%20urination%2C%20and%20headache.
	tributyl(methyl)phosphonium dimethyl phosphate	Skin and eye irritation are the main concerns associated with this compound.	https://pubchem.ncbi.nlm.nih.gov/compound/Tributyl_methyl_phosphonium-dimethyl-phosphate#section=Other-Identifiers
	amino trimethylene phosphonic acid	potential for skin and eye irritation.	https://www.parchem.com/siteimages/attachment/ghs%20amino%20trimethylene%20phosphonic%20acid%20msds.pdf
	P,P'-didi-phosphonic acid having phosphonic acid groups	Limited data	
	a polymer film of *N, N,* N', N'-ethylene-diamine-tetra-kis (methylene-phosphonic acid)-poly(ethylene oxide)	Skin sensitizer; potential for allergic reactions.	https://www.thfine.com/Ethylene-Diamine-Tetra-Methylene-Phosphonic-Acid-Sodium-Salt-pd6095416.html#:~:text=Package%20and%20Storage:,once%20contacted%2C%20flush%20with%20water.
epoxy resin	epoxy resin-based polymers containing diglycidyl ether bisphenol A, n-octylamine, and m-xylylenediamine	Limited data	
Polymeric materials	poly(acrylic acid) chains cross-linked with methylene-bisacrylamide, employing azobisisobutyronitrile phosphate	Limited data	
	poly-(acrylic acid) with carbonyl groups and tributyl (methyl) phosphonium dimethyl phosphate with phosphate groups	Limited data	
Graphene based materials	sulfonated graphene aerogels blended with polydimethylsiloxane	Limited data	
Acrylate-Based Materials	Benzyl acrylate (BzA	Skin and eye irritant; harmful if inhaled.	https://pubchem.ncbi.nlm.nih.gov/compound/Benzyl-acrylate
	Butyl acrylate	The main hazard of BA is its ability to irritate skin, eyes, and respiratory tract upon contact or inhalation.	[5]
Calcium Phosphate-Based Materials	$(Ca_{10}(PO_4)_6(OH)_2)$ Calcium hydroxyapatite or	It can cause irritation to the eyes and skin, and may irritate the respiratory tract	https://www.ltschem.com/msds/Ca10(PO4)6(OH)2.pdf
Aromatic Solvents	chlorobenzene	It can affect the central nervous system, liver, kidneys, and other organ systems.	https://www.nj.gov/health/eoh/rtkweb/documents/fs/0379.pdf https://wwwn.cdc.gov/tsp/substances/ToxSubstance.aspx?toxid=87
Solvents	DMF	Exposure to DMF can cause liver damage, skin	https://www.cdc.gov/niosh/docs/

		problems, and other health issues	90-105/default.html https://www.epa.gov/sites/default/files/2016-09/documents/n-n-dimethylformamide.pdf
	DMSO	DMSO is a cryoprotectant that can cause serious side effects, including fatal arrhythmias, respiratory arrest, and seizures.	[6], [7]
Others	1,3-bis(2-vinylbenzyl)-1H-benzimidazolium chloride (VBN)	Limited data	
	2,2′-dihydroxy-4,4′-dimethoxy-5,5′-disulfobenzophenone disodium salt (BP-9)	Limited data	

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