

Supplementary Information

Perovskite Photovoltaics: Life-Cycle Assessment of Energy and Environmental Impacts

Jian Gong,^a Seth B. Darling^{b,c} and Fengqi You^{a*}

^a Northwestern University, Department of Chemical and Biological Engineering, 2145 Sheridan Road, Evanston, IL, 60208, USA

^b Argonne National Laboratory, Center for Nanoscale Materials, 9700 South Cass Avenue, Argonne, IL, 60439, USA

^c University of Chicago, Institute for Molecular Engineering, 5801 South Ellis Avenue, Chicago, IL, 60637, USA

* To whom all correspondence should be addressed. Phone: (847) 467-2943; Fax: (847) 491-3728; E-mail: you@northwestern.edu

This Supplementary Information file includes: (1) life cycle inventory analyses for nine constituents used in manufacturing the TiO₂ and ZnO perovskite solar modules, namely, PbI₂, CH₃NH₃I, spiro-OMeTAD, FTO glass, ITO glass, BL-TiO₂ ink, nc-TiO₂ ink, ZnO ink, and silver paste; (2) all life cycle impact assessment data from Ecoinvent database; (3) uncertainty analysis and sensitivity analysis for the energy payback time (EPBT) and the CO₂ emissions factor of the ZnO module.

1. Life cycle inventory analysis for unavailable raw materials

1.1 PbI₂

The manufacturing route for PbI₂ is shown in Figure S1. The process for manufacturing potassium iodide is derived based on a commercial process.¹ The lead nitrate production is based on the description of Carr.² The life cycle inventory and the corresponding life cycle impact assessment of 1 kg PbI₂ is shown in Table S1 and Table S2. In order to get the life cycle impact assessment results, the mass of the co-products is used to allocate the environmental impacts of the manufacturing process. Waste is treated with an incineration method. Note that water input and out is not listed in the inventory, but the corresponding heat consumption for distilled water is considered in the cumulative energy consumption.

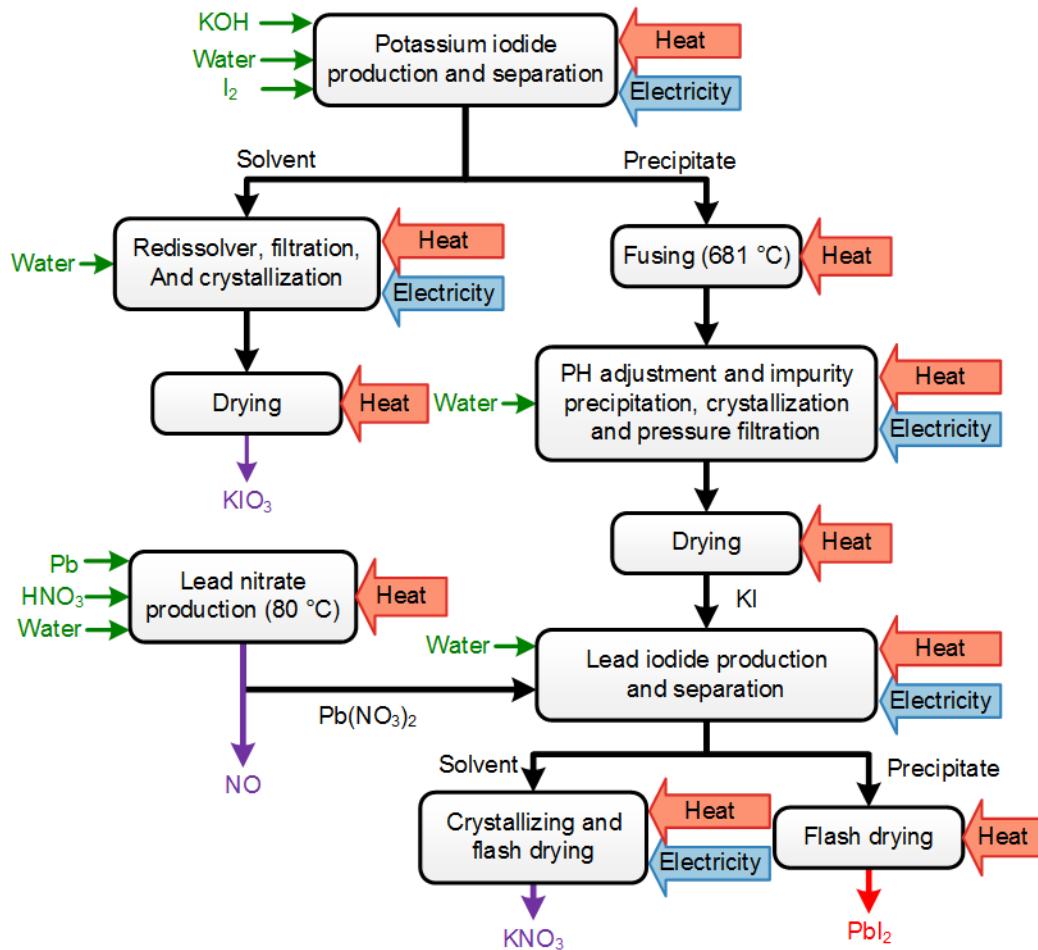


Figure S1. Manufacturing route for PbI_2 . Green flows represent feed materials, black flows represent intermediate products, purple flows represent co-products, the red flow represents major product. The numbers in the red and blue arrows are the heat and electricity consumption in MJ of the corresponding unit processes in order to produce one kg of the major product.

Table S1. Material and energy inventory of a PbI₂ manufacturing process

	Value	Unit
Process input		
Iodine (I ₂)	0.670	kg
Potassium hydroxide (KOH)	0.291	kg
Lead (Pb)	0.449	kg
Nitric acid (HNO ₃) ^a	0.729	kg
Cumulative heat consumption	13.5	MJ
Cumulative electricity consumption	0.133	kWh
Products		
Lead iodide (PbI ₂)	1.00	kg
Potassium nitrate (KNO ₃)	0.438	kg
Potassium iodate (KIO ₃)	0.135	kg
Nitric oxide (NO)	0.0434	kg
waste	0.160	kg

a. Commercially available nitric acid of 50 wt% is used.

Table S2. Life cycle impact assessment results for 1 kg PbI₂

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	3.44E-02	kg SO ₂ -Eq
Eutrophication potential	9.83E-03	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	1.42E+00	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	2.99E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	1.23E+00	kg 1,4-DCB-Eq
Ionising radiation	1.04E-08	DALYs
Land use	5.60E-01	m ² a
Malodours air	3.79E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	5.23E+00	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	5.50E+00	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	9.14E-04	kg formed ozone
Depletion of abiotic resources	4.90E-02	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	5.71E-07	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	1.23E-03	kg 1,4-DCB-Eq
Cumulative energy demand	6.56E+01	MJ-Eq
Climate change (IPCC 2013)	3.80E+00	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	9.01E-02	points
Eco-indicator 99 (human health)	3.09E-01	points
Eco-indicator 99 (resources)	4.25E-01	points

The first step to manufacture PbI₂ in Figure S1 is shown in Figure S2, and we use this step as an example to elaborate how the inventory analysis is performed. This step involves a chemical reaction shown in (S1). The input materials are potassium hydroxide (KOH), water, and iodine (I₂), while the output consists of a precipitate product and a solvent product. The precipitate product is primarily made of potassium iodate (KIO₃), and the minor constituents include water and solid waste. In contrast, the solvent product is made of potassium iodide (KI), dissolvable

waste, and water. The process consumes heat to generate distilled water and electricity to perform separations.

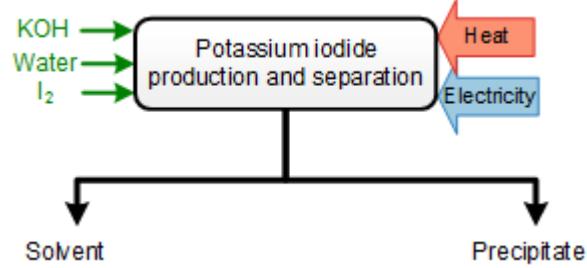


Figure S2. The first step to manufacture PbI₂.



$$M_{I_2} = M_{I_2-\text{impure}} + M_{I_2-\text{pure}} \quad (\text{S2})$$

$$M_{I_2-\text{impure}} = con_{I_2-KI} \cdot M_{KI} \quad (\text{S3})$$

$$M_{I_2-\text{pure}} = sc_{I_2-KI} \cdot M_{KI} \quad (\text{S4})$$

$$M_{KOH} = sc_{KOH-KI} \cdot M_{KI} \quad (\text{S5})$$

$$M_{water} = \alpha \cdot sol_{KOH} \cdot M_{KOH} \quad (\text{S6})$$

$$M_{KIO_3} = sc_{KIO_3-KI} \cdot M_{KI} - sol_{KIO_3} \cdot (M_{water} + sc_{water} \cdot M_{KI}) \quad (\text{S7})$$

The mass and energy in the inventory is evaluated by Equations (S2)-(S9). The mass of KI is set as 1 kg. In Equation (S2), the mass of raw material I₂ is the sum of the mass of the impurities and pure I₂. According to the U.S. Environmental Protection Agency,¹ the impurities from raw iodine amount to 15 kg/kkg (*con_{I₂-KI}*) of the KI product in (S3). The mass of the pure I₂ and KOH are calculated based on the stoichiometric relationship (*sc_{I₂-KI}* and *sc_{KOH-KI}*) in (S4) and (S5), respectively. The mass of water in (S6) is based on the solubility of KOH at 20 °C, which is 1.12 g KOH/g water (*sol_{KOH}*). $\alpha=2$ is a coefficient to ensure that all the KI is dissolved in the solvent product. In Equation (S7), the mass of KIO₃ in the precipitate product equals the stoichiometric mass (*sc_{KIO₃-KI}*) of KIO₃ minus the dissolved KIO₃ (*sol_{KIO₃}*). The solid waste comes from the impurities, while the water content is twice the volume of the precipitate.³ The remaining products are left in the solvent. Additionally, the heat and electricity consumption are determined by Equations (S8) and (S9), respectively. Δh_{water} represents the heat of vaporization of water, while $uc_{filter} = 0.21 \text{ MJ/kg solid}$ is the unit electricity consumption of a pressure filter.³

$$E_{heat} = \Delta h_{water} \cdot M_{water} \quad (\text{S8})$$

$$E_{electricity} = uc_{filter} \cdot M_{KIO_3} \quad (S9)$$

The inventory of this step is shown in Table S3.

Table S3. Mass and energy inventory of the first step to in the PbI₂ manufacturing process

	Values	Units
Process input		
Iodine (I ₂)	0.933	kg
Potassium hydroxide (KOH)	0.405	kg
Water	0.800	kg
Heat consumption	1.72	MJ
Electricity consumption	0.0119	kWh
Products		
Precipitate	0.188 0.0966 0.0135	kg kg kg
Solvent	1.00 0.768 0.0714	kg kg kg

We conduct inventory analysis for each step in the process of manufacturing PbI₂. We integrate the results in each step and finally obtain life cycle inventory and the corresponding life cycle impact assessment of 1 kg PbI₂ is shown in Table S1 and Table S2.

1.2 CH₃NH₃I

The manufacturing route for CH₃NH₃I is shown in Figure S3. The process for manufacturing 57% hydriodic acid is derived from the Rhodium Archive.⁴ The life cycle inventory and the corresponding life cycle impact assessment of 1 kg CH₃NH₃I is shown in Table S4 and Table S5. In order to get the life cycle impact assessment results, the mass of the co-products is used to allocate the environmental impacts of the manufacturing process. Waste is treated with an incineration method. Note that water input and out is not listed in the inventory, but the

corresponding heat consumption for distilled water is considered in the cumulative energy consumption.

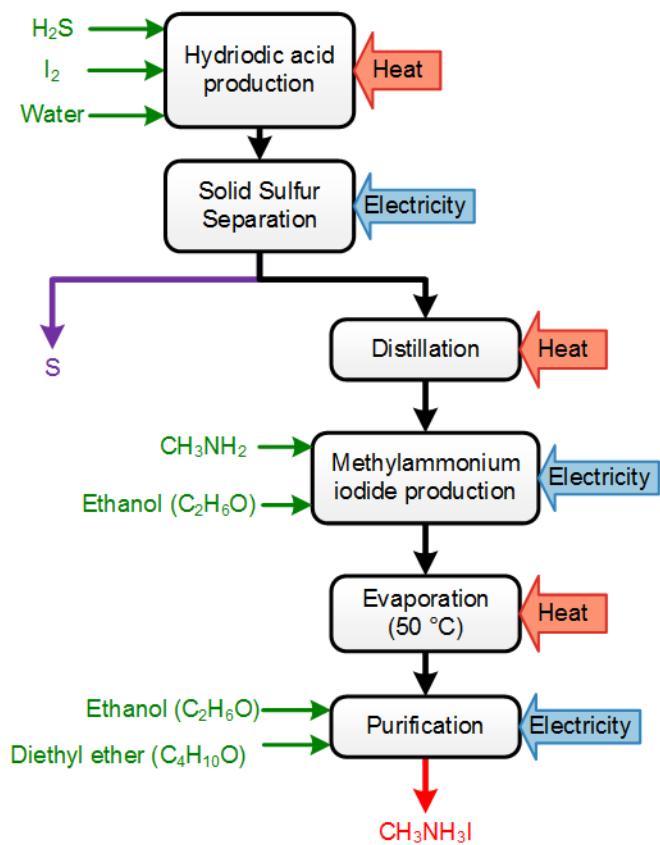


Figure S3. The manufacturing route for $\text{CH}_3\text{NH}_3\text{I}$. The representations follow the same manner of Figure S1.

Table S4. Material and energy inventory of a $\text{CH}_3\text{NH}_3\text{I}$ manufacturing process

	Value	Unit
Process input		
Hydrogen sulfide (H_2S)	0.139	kg
Iodine (I_2)	1.04	kg
Methylamine (CH_3NH_2)	0.581	kg
Ethanol ($\text{C}_2\text{H}_6\text{O}$)	7.31	kg
Diethyl ether ($\text{C}_4\text{H}_{10}\text{O}$)	20.8	kg
Cumulative heat consumption	8.30	MJ
Cumulative electricity consumption	9.24	kWh
Products		
Methylammonium iodide ($\text{CH}_3\text{NH}_3\text{I}$)	1.00	kg
Sulfur (S)	0.118	kg
Waste	29.9	kg

Table S5. Life cycle impact assessment results for 1 kg $\text{CH}_3\text{NH}_3\text{I}$

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	1.64E+00	kg $\text{SO}_2\text{-Eq}$
Eutrophication potential	5.86E-01	kg $\text{PO}_4\text{-Eq}$
Freshwater aquatic ecotoxicity (FAETP 100a)	1.19E+02	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	2.70E+02	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	8.10E+01	kg 1,4-DCB-Eq
Ionising radiation	6.09E-07	DALYs
Land use	1.79E+01	m^2a
Malodours air	1.64E+06	$\text{m}^3 \text{air}$
Marine aquatic ecotoxicity (MAETP 100a)	4.13E+02	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	4.73E+02	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	1.50E-01	kg formed ozone
Depletion of abiotic resources	1.75E+00	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	9.13E-05	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	1.19E-01	kg 1,4-DCB-Eq
Cumulative energy demand	3.96E+03	MJ-Eq
Climate change (IPCC 2013)	1.36E+02	kg $\text{CO}_2\text{-Eq}$
Eco-indicator 99 (ecosystem quality)	4.34E+01	points
Eco-indicator 99 (human health)	1.56E+01	points
Eco-indicator 99 (resources)	8.88E+00	points

1.3 Spiro-OMeTAD

The manufacturing routes for spiro-OMeTAD are shown in Figure S4 and Figure S5. The processes for manufacturing anisole,⁵ 4-iodoanisole,⁶ p-anisidine,⁷ phenylhydrazine,⁸ 2-aminobiphenyl,⁹ fluorene,¹⁰ and 9-fluorenone¹¹ are found in the literature. The routes for producing spiro-OMeTAD from these materials are specified in Yuan's thesis.¹² The life cycle inventory and the corresponding life cycle impact assessment of 1 kg spiro-OMeTAD is shown in Table S6 and Table S7. In order to get the life cycle impact assessment results, the mass of the co-products is used to allocate the environmental impacts of the manufacturing process. Waste is treated with an incineration method. Note that water input and out is not listed in the inventory, but the

corresponding heat consumption for distilled water is considered in the cumulative energy consumption.

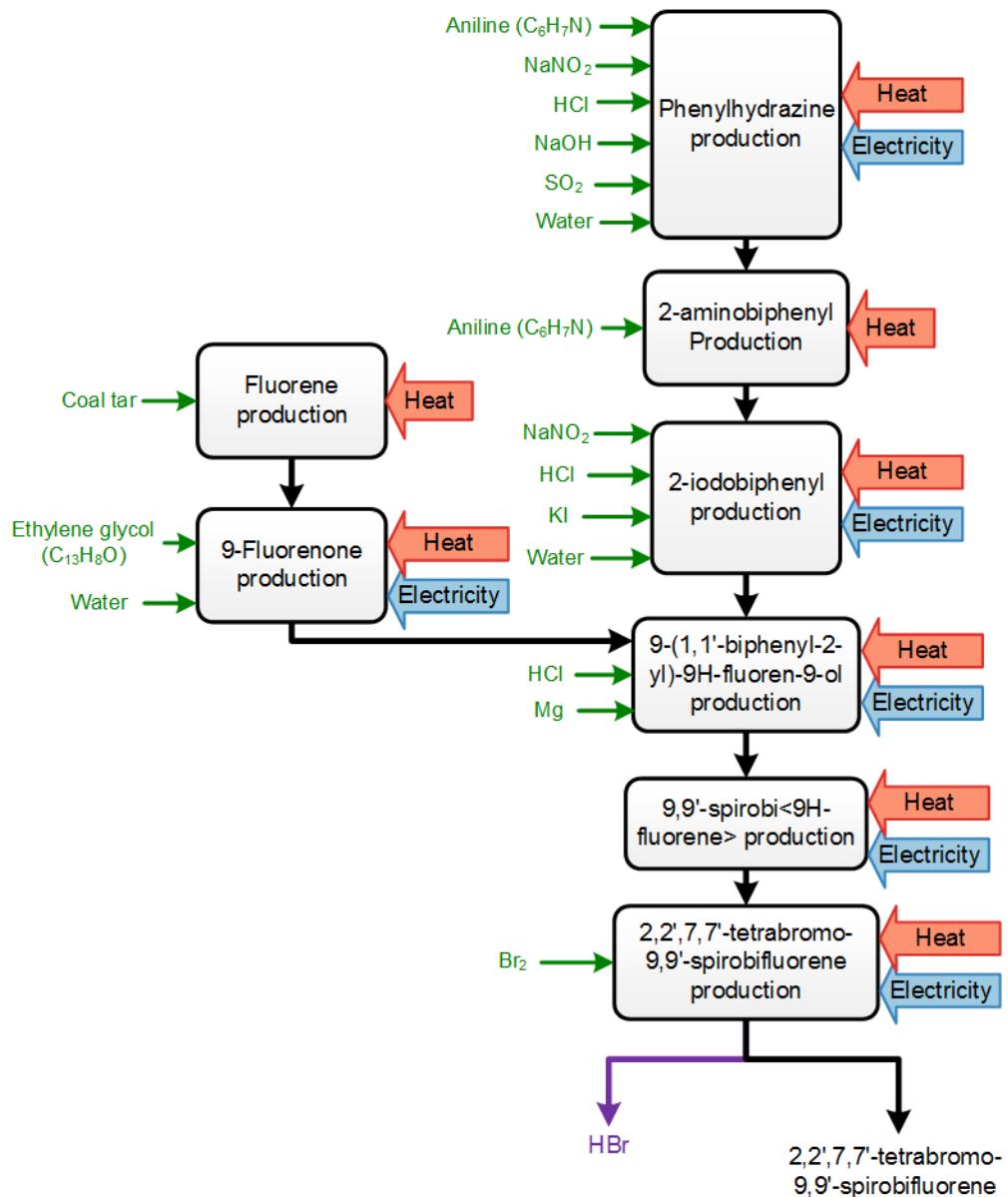


Figure S4. Part A of the manufacturing route for spiro-OMeTAD. The representations follow the same manner of Figure S1.

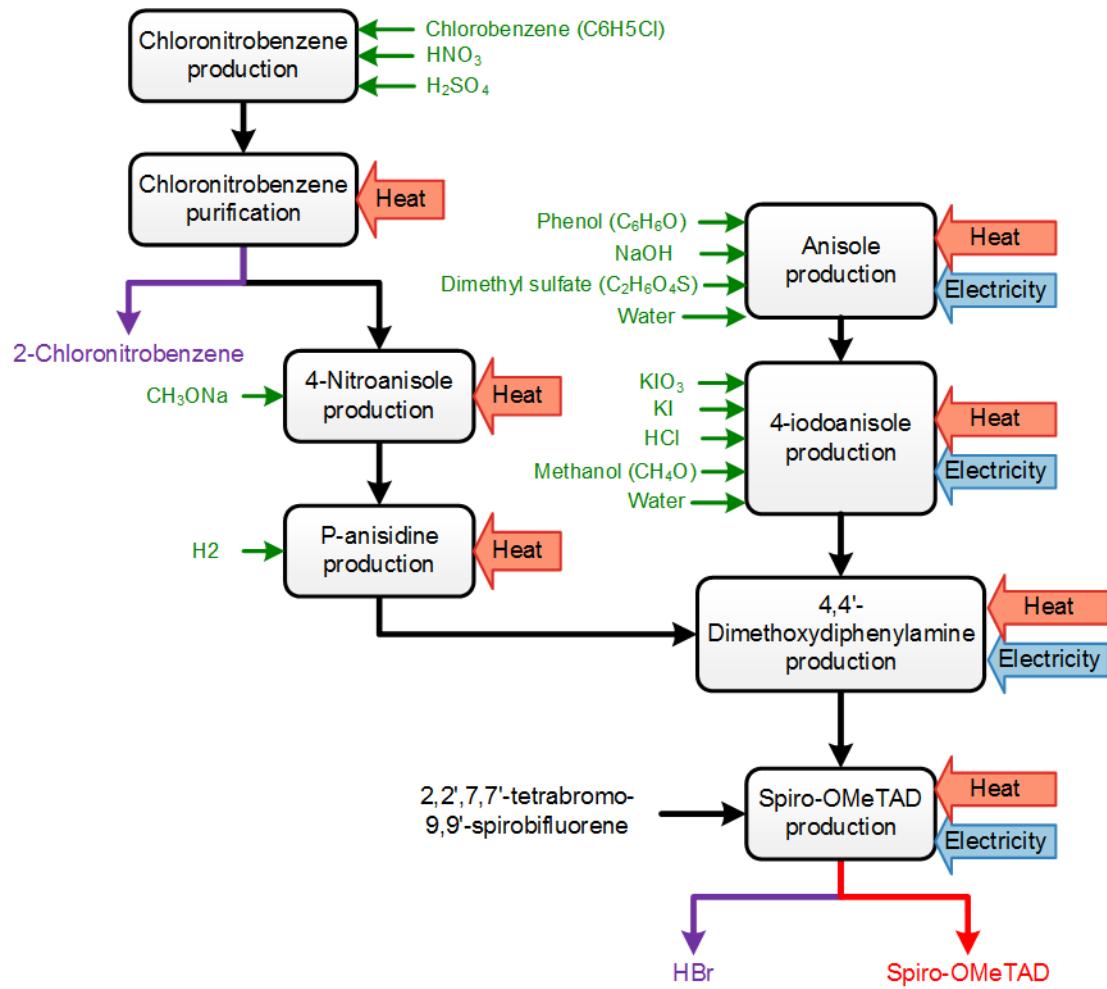


Figure S5. Part B of the manufacturing route for spiro-OMeTAD. The representations follow the same manner of Figure S1.

Table S6. Material and energy inventory of a spiro-OMeTAD manufacturing process

	Value	Unit
Process input		
Phenol (C_6H_6O)	0.724	kg
Sodium hydroxide (NaOH)	1.63	kg
Dimethyl sulfate ($C_2H_6O_4S$)	0.485	kg
Potassium iodide (KI)	0.837	kg
Potassium iodate (KIO_3)	0.412	kg
Methanol (CH_4O)	2.47	kg
Hydrogen chloride (HCl) ^a	5.04	kg
Hydrogen (H_2)	0.0295	kg
Sodium methoxide (CH_3ONa)	0.279	kg
Chlorobenzene (C_6H_5Cl)	0.966	kg
Nitric acid (HNO_3) ^b	1.08	kg
Sulfuric acid (H_2SO_4)	1.62	kg
Bromine (Br_2)	0.604	kg
Coal tar	0.295	kg
Ethylene glycol (C_2H_6O)	1.06	kg
Aniline ($C_6H_5NH_2$)	0.944	kg
Sodium nitrite ($NaNO_2$)	0.221	kg
Sulfur dioxide (SO_2)	0.407	kg
Magnesium (Mg)	0.0267	kg
Cumulative heat consumption	272	MJ
Cumulative electricity consumption	24.3	kWh
Products		
Spiro-OMeTAD ($C_{81}H_{88}N_4O_8$)	1.00	kg
Hydrogen bromide (HBr)	0.567	kg
2-Chloronitrobenzene ($C_6H_4ClNO_2$)	0.428	kg
Waste	81.9	kg

a. Commercially available hydrogen chloride of 30 wt% is used.

b. Commercially available nitric acid of 50 wt% is used.

Table S7. Life cycle impact assessment results for 1 kg spiro-OMeTAD

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	5.22E-01	kg SO_2 -Eq
Eutrophication potential	5.68E-01	kg PO_4 -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	1.64E+02	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	3.95E+02	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	2.04E+02	kg 1,4-DCB-Eq
Ionising radiation	2.37E-07	DALYs
Land use	3.90E+00	m^2 ^a
Malodours air	1.14E+06	m^3 air
Marine aquatic ecotoxicity (MAETP 100a)	5.53E+02	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	6.73E+02	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	1.35E-02	kg formed ozone
Depletion of abiotic resources	8.01E-01	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.60E-05	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	1.96E-02	kg 1,4-DCB-Eq

Cumulative energy demand	1.59E+03	MJ-Eq
Climate change (IPCC 2013)	9.68E+01	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	1.74E+00	points
Eco-indicator 99 (human health)	7.06E+00	points
Eco-indicator 99 (resources)	3.73E+00	points

1.4 FTO glass

The life cycle inventory of manufacturing 1 kg FTO glass is shown in Table S8, which is extracted from a paper by Syrrakon *et al.*¹³ Based on the life cycle inventory, we derive the corresponding life cycle impact assessment results, shown in Table S9.

Table S8. Material and energy inventory of manufacturing 1 kg FTO glass¹³

	Values	Units
Raw material		
Silica sand	7.88E-01	kg
Soda ash	2.86E-01	kg
Limestone	1.41E-01	kg
Dolomite	9.10E-02	kg
Alumina	4.30E-02	kg
Cullet	1.10E-02	kg
Tin	5.01E-03	kg
Chloride	5.99E-03	kg
Heat consumption	7.88E-01	MJ
Air emissions		
Carbon dioxide	1.28E-01	kg
Nitrogen oxide	3.00E-03	kg
Sulphur oxide	2.30E-03	kg
Methane	8.15E-04	kg
Particulates	1.00E-04	kg
Hydrogen fluoride	2.65E-05	kg
Lead	2.22E-05	kg
Arsenic	5.00E-06	kg
Nickel	5.56E-07	kg
Water emissions		
Chloride	8.20E-02	kg
COD	2.31E-04	kg
Sulfate	1.80E-04	kg
Suspended Solids	5.33E-05	kg
Fluoride	4.44E-05	kg
Mineral oil	3.56E-05	kg
Ammonia	1.78E-05	kg
Boric acid	7.11E-06	kg
Barium	5.33E-06	kg
Phenol	1.78E-06	kg
Chromium, Copper, tin, lead, nickel, zinc	8.89E-07	kg
Arsenic, antimony	5.33E-07	kg
Cadmium	5.00E-07	kg
Solid waste	6.82E-02	kg

Table S9. Life cycle impact assessment results for 1 kg FTO glass

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	8.66E-02	kg SO ₂ -Eq
Eutrophication potential	2.04E-03	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	6.34E-01	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	1.47E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	1.33E+00	kg 1,4-DCB-Eq
Ionising radiation	1.58E-09	DALYs
Land use	3.98E-02	m ² a
Malodours air	2.67E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	2.32E+00	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	2.63E+00	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	1.29E-04	kg formed ozone
Depletion of abiotic resources	1.11E-02	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.13E-07	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	3.37E-04	kg 1,4-DCB-Eq
Cumulative energy demand	2.51E+01	MJ-Eq
Climate change (IPCC 2013)	1.33E+00	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	1.65E-02	points
Eco-indicator 99 (human health)	7.94E-02	points
Eco-indicator 99 (resources)	1.83E-01	points

1.5 ITO glass

As opposed to FTO glass, ITO glass is employed in the ZnO module. We extract the life cycle inventory of 1 m² ITO glass from a paper by Garcia-Valverde *et al.*¹⁴ and present the information in Table S10. Accordingly, we calculate the impact indicators of the ITO and show them in Table S11.

Table S10. Material and energy inventory of manufacturing 1 m² ITO glass¹⁴

	Values	Units
Indium (In)	2.30E-03	kg
Tin (Sn)	2.00E-04	kg
Glass	1.54E+00	kg
Titanium dioxide (SiO ₂)	1.00E-04	kg
Argon (Ar)	1.24E-01	kg
Oxygen (O ₂)	1.00E-04	kg
Electricity consumption	2.25E+01	kWh

Table S11. Life cycle impact assessment results for 1 m² ITO glass

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	1.19E-01	kg SO ₂ -Eq
Eutrophication potential	2.91E-02	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	4.62E+00	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	9.64E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	4.67E+00	kg 1,4-DCB-Eq
Ionising radiation	1.20E-07	DALYs

Land use	1.01E+00	m ² a
Malodours air	3.78E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	1.67E+01	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	1.70E+01	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	9.10E-04	kg formed ozone
Depletion of abiotic resources	1.44E-01	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	8.56E-07	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	3.26E-03	kg 1,4-DCB-Eq
Cumulative energy demand	3.14E+02	MJ-Eq
Climate change (IPCC 2013)	1.54E+01	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	2.17E-01	points
Eco-indicator 99 (human health)	4.11E-01	points
Eco-indicator 99 (resources)	6.16E-01	points

1.6 BL-TiO₂ ink

The blocking-layer TiO₂ ink (BL-TiO₂ ink) is prepared according to Kavan's method.¹⁵ The corresponding life cycle inventory is summarized in Table S12 and the corresponding life cycle impact assessment results are shown in Table S13.

Table S12. Material and energy inventory of 1 kg BL-TiO₂ ink

	Value	Unit
Titanium tetrachloride (TiCl ₄)	4.81E-02	kg
Isopropanol (C ₃ H ₈ O)	6.08E-02	kg
Acetone (C ₃ H ₆ O)	2.94E-02	kg
Acetic anhydride (C ₄ H ₆ O ₃)	5.18E-02	kg
Ethanol (C ₂ H ₆ O)	9.08E-01	kg
Heat consumption	1.54E-03	MJ
Electricity consumption	7.04E-05	kWh

Table S13. Life cycle impact assessment results for 1 kg BL-TiO₂ ink

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	1.22E-02	kg SO ₂ -Eq
Eutrophication potential	6.07E-03	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	6.25E-01	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	1.15E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	5.17E-01	kg 1,4-DCB-Eq
Ionising radiation	3.19E-09	DALYs
Land use	1.06E+00	m ² a
Malodours air	2.96E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	1.65E+00	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	1.83E+00	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	6.98E-04	kg formed ozone
Depletion of abiotic resources	1.28E-02	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.37E-07	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	6.18E-03	kg 1,4-DCB-Eq
Cumulative energy demand	4.97E+01	MJ-Eq

Climate change (IPCC 2013)	1.54E+00	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	5.09E+00	points
Eco-indicator 99 (human health)	7.62E-02	points
Eco-indicator 99 (resources)	6.52E-02	points

1.7 nc-TiO₂ ink

The nanocrystalline TiO₂ (nc-TiO₂) ink is assumed a mixture of Titanium dioxide and terpineol according to commercial products.¹⁶ The life cycle inventory of the nc-TiO₂ ink is shown in Table S14 and the life cycle impact assessment results are shown in Table S15.

Table S14. Material and energy inventory of 1 kg nc-TiO₂ ink

	Value	Unit
Titanium dioxide (TiO ₂)	0.153	kg
Terpineol (C ₁₀ H ₁₈ O)	0.847	kg

Table S15. Life cycle impact assessment results for 1 kg nc-TiO₂ ink

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	1.22E-02	kg SO ₂ -Eq
Eutrophication potential	6.07E-03	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	6.25E-01	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	1.15E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	5.17E-01	kg 1,4-DCB-Eq
Ionising radiation	3.19E-09	DALYs
Land use	1.06E+00	m ² a
Malodours air	2.96E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	1.65E+00	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	1.83E+00	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	6.98E-04	kg formed ozone
Depletion of abiotic resources	1.28E-02	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.37E-07	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	6.18E-03	kg 1,4-DCB-Eq
Cumulative energy demand	4.97E+01	MJ-Eq
Climate change (IPCC 2013)	1.54E+00	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	5.09E+00	points
Eco-indicator 99 (human health)	7.62E-02	points
Eco-indicator 99 (resources)	6.52E-02	points

1.8 ZnO ink

The ZnO ink is prepared following the method by Liu *et al.*¹⁷ The corresponding material and energy inventory and life cycle impact assessment results of 1 kg ZnO ink are shown in Table S16 and Table S17, respectively.

Table S16. Material and energy inventory of 1 kg ZnO ink

	Values	Units
Zinc oxide (ZnO)	7.13E-03	kg
Acetic acid (C ₂ H ₄ O ₂)	1.05E-02	kg
Hydrogen peroxide (H ₂ O ₂) ^a	8.00E-05	kg

Potassium hydroxide (KOH)	9.64E-03	kg
n-Butanol (C ₄ H ₁₀ O)	8.27E-01	kg
Methanol (CH ₄ O)	1.24E+00	kg
Chloroform (CHCl ₃)	1.08E-01	kg
Waste	3.35E-02	kg
Heat consumption	1.40E+00	MJ
Electricity consumption	4.11E+00	kWh

a. Commercially available hydrogen peroxide of 50 wt% is used.

Table S17. Life cycle impact assessment results for 1 kg ZnO ink

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	4.13E-02	kg SO ₂ -Eq
Eutrophication potential	8.88E-03	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	1.65E+00	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	3.49E+00	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	1.74E+00	kg 1,4-DCB-Eq
Ionising radiation	2.75E-08	DALYs
Land use	3.22E-01	m ² a
Malodours air	8.52E+04	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	5.79E+00	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	6.13E+00	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	4.47E-03	kg formed ozone
Depletion of abiotic resources	7.95E-02	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.36E-04	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	8.11E-04	kg 1,4-DCB-Eq
Cumulative energy demand	1.71E+02	MJ-Eq
Climate change (IPCC 2013)	5.74E+00	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	5.39E-02	points
Eco-indicator 99 (human health)	2.55E-01	points
Eco-indicator 99 (resources)	3.97E-01	points

1.9 Silver paste

The silver paste used in the TiO₂ module consists of 70% silver powder and 30% thinner, which is butyl acetate.¹⁸ The silver powder is prepared following a US patent by Irizarry and Yang.¹⁹ We show the life cycle inventory and life cycle impact assessment results in Table S18 and Table S19, respectively.

Table S18. Material and energy inventory of 1 kg silver paste

	Values	Units
Process input		
Silver solid	7.00E-01	kg
Nitric acid (HNO ₃) ^a	2.02E+00	kg
Reducing agent (C ₇ H ₁₄)	8.82E-01	kg
Butyl acetate (C ₆ H ₁₂ O ₂)	3.00E-01	kg
Emissions		kg
Nitrogen dioxide (NO ₂)	2.99E-01	kg

a. Commercially available nitric acid of 50 wt% is used.

Table S19. Life cycle impact assessment results for 1 kg silver paste

Impact categories/ Endpoint indicators	Values	Units
Acidification potential	2.65E+00	kg SO ₂ -Eq
Eutrophication potential	1.41E+01	kg PO ₄ -Eq
Freshwater aquatic ecotoxicity (FAETP 100a)	3.69E+03	kg 1,4-DCB-Eq
Freshwater sediment ecotoxicity (FSETP 100a)	7.03E+03	kg 1,4-DCB-Eq
Human toxicity (HTP 100a)	1.69E+02	kg 1,4-DCB-Eq
Ionising radiation	1.24E-07	DALYs
Land use	1.81E+01	m ² a
Malodours air	9.74E+05	m ³ air
Marine aquatic ecotoxicity (MAETP 100a)	1.25E+04	kg 1,4-DCB-Eq
Marine sediment ecotoxicity (MSETP 100a)	1.19E+04	kg 1,4-DCB-Eq
Photochemical oxidation (EBIR)	5.47E-03	kg formed ozone
Depletion of abiotic resources	1.90E+00	kg antimony-Eq
Stratospheric ozone depletion (ODP 10a)	1.20E-05	kg CFC-11-Eq
Terrestrial ecotoxicity (TAETP 100a)	1.55E-01	kg 1,4-DCB-Eq
Cumulative energy demand	1.56E+03	MJ-Eq
Climate change (IPCC 2013)	8.23E+01	kg CO ₂ -Eq
Eco-indicator 99 (ecosystem quality)	2.24E+01	points
Eco-indicator 99 (human health)	2.26E+02	points
Eco-indicator 99 (resources)	3.79E+00	points

2. Characterization factors from Ecoinvent

In Table S20 and Table S21, we show all the characterization factors we extract from Ecoinvent database and use to evaluate the above constituents of the two types of perovskite solar modules.²⁰ The characterization factors for coproduced precious metals, such silver and gold, are calculated using the market prices-based allocation method.

Table S20. Characterization factors used in the evaluation part I

item	value	unit	acidification	eutrophication	freshwater aquatic ecotoxicity	freshwater sediment ecotoxicity	human toxicity	ionising radiation	land use	malodours air	marine aquatic ecotoxicity
electricity	1	kWh	4.31E-03	1.11E-03	1.76E-01	3.70E-01	1.70E-01	5.17E-09	4.02E-02	7.37E+02	6.25E-01
heat	1	MJ	2.39E-04	8.92E-06	2.95E-03	6.61E-03	9.09E-03	9.54E-12	1.07E-04	1.82E+03	1.10E-02
Iodine (I2)	1	kg	2.69E-02	5.39E-03	8.68E-01	1.87E+00	1.18E+00	7.93E-09	1.13E-01	3.18E+04	3.38E+00
potassium hydroxide (KOH)	1	kg	1.50E-02	3.62E-03	7.31E-01	1.59E+00	8.24E-01	6.72E-09	1.60E-01	1.87E+04	2.65E+00
lead (Pb)	1	kg	2.52E-02	8.51E-03	1.04E+00	2.10E+00	6.79E-01	7.31E-09	6.26E-01	1.39E+04	3.79E+00
nitric acid (HNO3) (50%)	1	kg	1.16E-02	4.43E-03	2.11E-01	4.70E-01	4.85E-01	8.58E-10	2.17E-02	1.64E+04	1.10E+00
hydrogen sulfide (H2S)	1	kg	2.69E-03	1.10E-03	2.27E-01	4.98E-01	2.92E-01	1.74E-09	3.06E-02	3.38E+03	8.10E-01
methylamine (CH3NH2)	1	kg	2.09E-02	4.42E-03	5.93E-01	1.23E+00	1.11E+00	4.81E-09	7.30E-02	8.84E+04	3.20E+00
ethanol (C2H6O)	1	kg	1.03E-02	5.70E-03	4.63E-01	7.49E-01	4.22E-01	2.47E-09	1.14E+00	1.42E+04	1.02E+00
diethyl ether (C4H10O)	1	kg	7.00E-02	1.70E-02	2.85E+00	6.09E+00	2.94E+00	2.52E-08	4.12E-01	6.55E+04	1.03E+01
phenol (C6H6O)	1	kg	1.80E-02	6.04E-03	9.31E-01	2.01E+00	1.39E+01	4.97E-09	1.12E-01	5.25E+04	3.38E+00
sodium hydroxide (NaOH) (50%)	1	kg	8.70E-03	2.44E-03	4.72E-01	1.03E+00	4.94E-01	4.90E-09	7.31E-02	9.32E+03	1.70E+00
dimethyl sulfate (C2H6O4S)	1	kg	1.73E-02	4.09E-03	7.41E-01	1.56E+00	8.41E-01	4.29E-09	8.27E-02	4.17E+04	2.60E+00
Potassium iodide (KI)	1	kg	2.85E-02	6.39E-03	1.21E+00	2.68E+00	1.35E+00	8.99E-09	1.49E-01	4.57E+04	4.50E+00
Potassium iodate (KIO3)	1	kg	3.19E-02	6.54E-03	1.26E+00	2.80E+00	1.48E+00	9.13E-09	1.51E-01	7.17E+04	4.69E+00
methanol (CH4O)	1	kg	6.49E-03	5.48E-04	1.63E-01	2.95E-01	1.14E-01	5.78E-10	6.10E-03	5.06E+04	4.95E-01
hydrochloric acid (HCl) (30%)	1	kg	1.15E-02	3.24E-03	6.84E-01	1.49E+00	7.61E-01	6.33E-09	1.00E-01	1.17E+04	2.45E+00
sulfuric acid (H2SO4)	1	kg	7.24E-03	3.69E-04	1.02E-01	2.26E-01	1.66E-01	7.06E-10	1.11E-02	3.14E+03	3.68E-01
chlorobenzene (C6H5Cl)	1	kg	1.68E-02	1.46E-02	9.74E-01	2.06E+00	2.16E+02	5.42E-09	1.27E-01	1.31E+04	3.41E+00
sodium methoxide (CH3ONa)	1	kg	3.96E-03	1.26E-03	1.88E-01	4.02E-01	1.67E-01	2.41E-09	2.78E-02	6.41E+03	6.73E-01
hydrogen (H2)	1	kg	1.12E-01	3.14E-02	6.08E+00	1.32E+01	6.36E+00	6.31E-08	9.41E-01	1.20E+05	2.19E+01
aniline (C6H7N)	1	kg	3.06E-02	9.07E-03	1.21E+00	2.61E+00	3.62E+00	5.79E-09	1.39E-01	2.70E+04	4.81E+00
sodium nitrite (NaNO2)	1	kg	1.90E-02	6.36E-03	9.13E-01	1.99E+00	1.25E+00	9.66E-09	1.27E-01	2.74E+04	3.84E+00
sulfur dioxide (SO2)	1	kg	5.09E-02	9.52E-04	2.25E-01	4.96E-01	3.26E-01	2.60E-09	2.93E-02	9.28E+03	8.25E-01
coal tar	1	kg	4.34E-03	1.17E-03	2.76E-01	6.05E-01	3.26E-01	2.27E-09	3.71E-02	5.47E+03	9.85E-01
ethylene glycol (C2H6O2)	1	kg	7.85E-03	2.33E-03	4.54E-01	9.91E-01	7.29E-01	3.83E-09	5.95E-02	1.12E+04	1.61E+00
magnesium (Mg)	1	kg	6.31E-02	8.39E-03	9.37E-01	2.03E+00	3.76E+00	8.33E-09	1.32E-01	6.14E+05	3.55E+00
bromine (Br2)	1	kg	2.73E-02	5.43E-03	8.80E-01	1.89E+00	1.19E+00	7.97E-09	1.14E-01	3.21E+04	3.42E+00
zinc oxide (ZnO)	1	kg	7.32E-03	1.25E-03	3.92E-01	8.82E-01	5.74E-01	1.68E-09	3.95E-02	3.62E+04	1.93E+00
acetic acid (C2H4O2) (98%)	1	kg	1.30E-02	2.64E-03	5.72E-01	1.22E+00	6.52E-01	6.10E-09	8.30E-02	1.16E+05	2.04E+00
hydrogen peroxide (H2O2) (50%)	1	kg	6.84E-03	1.66E-03	6.92E-01	1.43E+00	3.67E+00	2.66E-09	6.38E-02	1.23E+04	2.44E+00
n-Butanol (C4H10O)	1	kg	1.58E-02	3.27E-03	5.54E-01	1.20E+00	6.89E-01	5.60E-09	1.60E-01	1.30E+04	2.06E+00
chloroform (CHCl3)	1	kg	1.35E-02	3.13E-03	6.71E-01	1.47E+00	1.11E+00	6.05E-09	9.45E-02	3.34E+04	2.42E+00
Indium (In)	1	kg	2.64E+00	9.23E-01	1.88E+02	3.63E+02	2.51E+02	2.09E-07	1.05E+01	1.58E+06	7.73E+02
Tin (Sn)	1	kg	5.07E-01	5.10E-02	5.65E+00	1.23E+01	6.78E+00	7.36E-08	2.11E+00	1.25E+05	2.07E+01
glass	1	kg	9.84E-03	1.05E-03	1.06E-01	2.30E-01	1.49E-01	1.08E-09	4.80E-02	1.06E+04	4.05E-01
silica sand	1	kg	2.61E-04	4.88E-05	6.20E-03	1.34E-02	1.08E-02	4.11E-11	4.96E-03	5.88E+02	2.57E-02
argon (Ar)	1	kg	9.85E-03	3.56E-03	4.63E-01	9.91E-01	2.93E-01	7.94E-09	7.37E-02	9.13E+03	1.67E+00
oxygen (O2)	1	kg	4.49E-03	1.06E-03	1.74E-01	3.74E-01	1.25E-01	2.56E-09	2.86E-02	3.82E+03	6.31E-01
nitrogen (N2)	1	kg	4.35E-03	1.02E-03	1.68E-01	3.62E-01	1.21E-01	2.48E-09	2.77E-02	3.70E+03	6.11E-01
ethylene vinyl acetate	1	kg	8.46E-03	2.04E-03	3.62E-01	7.87E-01	4.39E-01	2.74E-09	5.22E-02	3.80E+04	1.28E+00
aluminium (Al)	1	kg	7.08E-02	1.10E-02	1.08E-01	2.55E+01	2.29E+01	8.19E-09	2.45E-01	5.87E+04	3.84E+01
Ilmenite	1	kg	3.84E-04	6.65E-05	7.08E-03	1.55E-02	1.47E-02	2.68E-10	3.02E-03	1.85E+02	3.13E-02
Iron pellet/powder	1	kg	1.22E-03	2.96E-04	3.25E-02	7.01E-02	3.89E-02	2.97E-10	5.25E-03	7.89E+02	1.22E-01
methane (CH4)	1	kg	7.76E-03	4.34E-03	3.40E-01	7.40E-01	8.68E-01	3.76E-09	7.92E+00	9.96E+03	1.14E+00
Gold (Au)	1	kg	2.03E-02	1.20E+03	3.14E+05	5.98E+05	1.41E+04	9.80E-06	1.50E-03	7.12E-07	1.06E+06
soda ash	1	kg	5.27E-03	2.64E-03	3.35E-01	7.37E-01	6.65E-01	2.36E-09	4.44E-02	1.24E+04	1.37E+00
limestone	1	kg	5.15E-05	1.39E-05	4.24E-04	9.31E-04	1.88E-03	5.09E-12	1.70E-04	2.13E+01	1.64E-03
dolomite	1	kg	3.05E-04	6.68E-05	9.72E-03	2.09E-02	1.12E-02	1.12E-10	3.03E-03	2.13E+02	3.61E-02
cullet	1	kg	3.94E-05	2.85E-05	1.70E-02	3.74E-02	4.71E-03	1.91E-11	8.37E-04	6.61E-01	5.76E-02
deionised water	1	kg	1.00E-05	3.55E-06	1.07E-03	2.48E-03	5.89E-04	7.01E-12	8.49E-05	1.25E+01	3.65E-03
chlorine (Cl2)	1	kg	8.43E-03	2.36E-03	4.58E-01	9.96E-01	4.78E-01	4.74E-09	7.08E-02	9.02E+03	1.65E+00

titanium dioxide (TiO2)	1	kg	4.52E-02	1.38E-02	6.73E+00	1.57E+01	2.31E+00	1.78E-08	5.23E-01	4.35E+04	2.37E+01
isopropanol (C3H8O)	1	kg	7.51E-03	4.32E-03	2.58E-01	5.60E-01	3.59E-01	1.17E-09	4.46E-02	9.97E+03	9.45E-01
acetone (C3H6O)	1	kg	1.02E-02	1.09E-03	2.86E-02	6.28E-02	7.84E-02	9.65E-12	5.04E-04	1.98E+02	1.22E-01
acetic anhydride (C4H6O3)	1	kg	2.19E-02	6.11E-03	9.97E-01	2.14E+00	1.22E+00	9.89E-09	2.18E-01	2.93E+05	3.62E+00
methylcyclohexane (C7H14)	1	kg	2.06E-02	3.81E-03	5.27E-01	1.13E+00	8.67E-01	2.71E-09	2.66E-01	2.81E+04	2.04E+00
butyl acetate (C6H12O2)	1	kg	2.04E-02	5.39E-03	8.88E-01	1.92E+00	1.14E+00	8.71E-09	2.37E-01	1.52E+05	3.27E+00
silver (Ag)	1	kg	3.42E+00	2.01E+01	5.27E+03	1.00E+04	2.36E+02	1.65E-07	2.53E+01	1.20E+06	1.78E+04
adhesive	1	kg	3.12E-03	6.57E-04	9.39E-02	2.04E-01	2.31E-01	2.40E-09	8.99E-02	5.98E+03	3.79E-01
dimethylformamide (C3H7NO)	1	kg	2.18E-02	9.30E-03	8.32E-01	1.76E+00	1.16E+00	7.78E-09	1.23E-01	9.99E+05	3.45E+00
PET	1	kg	1.34E-02	3.53E-03	6.84E-01	1.49E+00	1.15E+00	5.04E-09	1.32E-01	2.46E+04	2.58E+00
incineration of average residue	1	kg	1.15E-03	5.78E-03	1.81E+00	4.42E+00	4.51E-01	3.04E-10	1.82E-02	2.37E+03	6.06E+00
inert material landfill	1	kg	4.74E-05	9.03E-06	5.93E-04	1.32E-03	2.64E-03	1.65E-11	1.66E-03	7.82E+01	2.55E-03

Table S21. Characterization factors used in the evaluation part II

item	value	unit	marine sediment ecotoxicity	photochemical oxidation	depletion of abiotic resources	stratospheric ozone depletion	terrestrial ecotoxicity	cumulative energy demand (MJ-eq)	climate change (IPCC 2013)	Eco-indicator 99 (ecosystem quality)	Eco-indicator 99 (human health)	Eco-indicator 99 (resources)
electricity	1	kWh	6.34E-01	3.30E-05	5.72E-03	3.13E-08	7.16E-05	1.27E+01	6.12E-01	5.95E-03	1.24E-02	2.32E-02
heat	1	MJ	1.19E-02	4.97E-06	5.71E-04	3.32E-09	1.46E-06	1.17E+00	6.19E-02	6.65E-05	7.72E-04	3.13E-03
Iodine (I2)	1	kg	3.64E+00	6.13E-04	7.84E-02	1.07E-06	9.65E-04	7.14E+01	4.66E+00	3.06E-02	1.98E-01	1.73E-01
potassium hydroxide (KOH)	1	kg	2.87E+00	2.20E-04	1.61E-02	1.36E-07	4.52E-04	3.37E+01	1.90E+00	2.51E-02	2.20E-01	7.31E-02
lead (Pb)	1	kg	3.83E+00	7.78E-04	1.49E-02	1.34E-07	1.05E-03	3.04E+01	1.55E+00	9.32E-02	2.39E-01	4.18E-01
nitric acid (HNO3) (50%)	1	kg	1.22E+00	7.47E-05	6.09E-03	7.55E-08	5.48E-04	1.31E+01	3.02E+00	1.44E-02	4.77E-02	3.55E-02
hydrogen sulfide (H2S)	1	kg	8.99E-01	5.44E-05	5.09E-03	6.18E-08	1.43E-04	1.06E+01	4.03E-01	7.05E-03	3.60E-02	2.50E-02
methylamine (CH3NH2)	1	kg	3.46E+00	9.91E-04	3.45E-02	4.03E-07	1.83E-03	7.32E+01	2.17E+00	2.54E-02	1.08E-01	1.91E-01
ethanol (C2H6O)	1	kg	1.12E+00	1.74E-04	8.12E-03	8.41E-08	6.72E-03	4.19E+01	1.19E+00	5.61E+00	5.37E-02	4.02E-02
diethyl ether (C4H10O)	1	kg	1.10E+01	7.03E-03	7.22E-02	4.26E-06	3.06E-03	1.61E+02	5.02E+00	8.93E-02	6.42E-01	3.79E-01
phenol (C6H6O)	1	kg	3.65E+00	3.48E-03	5.69E-02	3.28E-07	4.09E-04	1.19E+02	3.97E+00	2.79E-02	1.87E-01	2.95E-01
sodium hydroxide (NaOH) (50%)	1	kg	1.85E+00	1.01E-04	8.71E-03	1.24E-06	2.89E-04	1.86E+01	1.03E+00	1.30E-02	1.47E-01	3.83E-02
dimethyl sulfate (C2H6O4S)	1	kg	2.81E+00	5.06E-04	1.83E-02	2.00E-07	3.31E-04	3.91E+01	7.96E-01	2.15E-02	1.28E-01	1.00E-01
Potassium iodide (KI)	1	kg	4.98E+00	6.00E-04	7.19E-02	9.17E-07	9.41E-04	7.77E+01	4.87E+00	3.55E-02	2.43E-01	1.87E-01
Potassium iodate (KIO3)	1	kg	5.19E+00	6.71E-04	8.00E-02	9.64E-07	9.62E-04	9.45E+01	5.76E+00	3.65E-02	2.55E-01	2.32E-01
methanol (CH4O)	1	kg	5.07E-01	2.35E-04	1.63E-02	1.40E-07	5.15E-05	3.36E+01	3.81E-01	2.57E-03	2.23E-02	8.96E-02
hydrochloric acid (HCl) (30%)	1	kg	2.68E+00	1.39E-04	1.22E-02	1.20E-06	6.48E-04	2.61E+01	1.38E+00	1.86E-02	1.95E-01	5.55E-02
sulfuric acid (H2SO4)	1	kg	4.16E-01	3.50E-05	3.17E-03	6.08E-08	5.02E-05	7.08E+00	-1.50E-01	4.31E-03	2.10E-02	1.90E-02
chlorobenzene (C6H5Cl)	1	kg	3.68E+00	2.30E-03	3.94E-02	1.26E-06	7.65E-04	7.99E+01	2.78E+00	2.83E-02	2.10E-01	1.93E-01
sodium methoxide (CH3ONa)	1	kg	7.21E-01	7.26E-05	4.53E-03	1.27E-07	1.57E-04	9.89E+00	4.40E-01	5.07E-03	5.67E-02	2.08E-02
hydrogen (H2)	1	kg	2.38E+01	1.30E-03	1.12E-01	1.60E-05	3.73E-03	2.40E+02	1.32E+01	1.67E-01	1.89E+00	4.93E-01
aniline (C6H7N)	1	kg	5.19E+00	8.27E-04	4.67E-02	4.41E-07	1.06E-03	9.65E+01	4.69E+00	4.34E-02	2.13E-01	2.42E-01
sodium nitrite (NaNO2)	1	kg	4.19E+00	2.76E-04	2.06E-02	9.80E-07	1.57E-03	4.52E+01	2.33E+00	3.18E-02	2.04E-01	1.02E-01
sulfur dioxide (SO2)	1	kg	9.19E-01	9.77E-05	9.59E-03	1.65E-07	1.40E-04	2.12E+01	-1.43E+00	1.13E-02	9.70E-02	5.39E-02
coal tar	1	kg	1.08E+00	5.33E-05	4.64E-03	3.53E-08	1.38E-04	9.84E+00	5.34E-01	7.17E-03	7.40E-02	2.14E-02
ethylene glycol (C2H6O2)	1	kg	1.77E+00	6.28E-04	2.32E-02	4.90E-08	2.43E-04	5.19E+01	1.62E+00	1.33E-02	1.01E-01	1.28E-01
magnesium (Mg)	1	kg	3.84E+00	3.32E-03	1.73E-01	5.51E-06	9.18E-04	3.56E+02	1.82E+01	4.32E-02	3.55E-01	9.37E-01
bromine (Br2)	1	kg	3.68E+00	6.15E-04	4.25E-02	1.08E-06	9.69E-04	7.18E+01	4.65E+00	3.09E-02	2.00E-01	1.75E-01
zinc oxide (ZnO)	1	kg	2.32E+00	1.94E-04	1.30E-02	1.25E-07	5.22E-04	2.70E+01	1.42E+00	1.30E-01	6.41E-02	7.01E-02
acetic acid (C2H4O2) (98%)	1	kg	2.22E+00	1.13E-03	2.43E-02	3.19E-07	3.39E-04	5.21E+01	1.48E+00	1.60E-02	1.52E-01	1.29E-01
hydrogen peroxide (H2O2) (50%)	1	kg	2.53E+00	1.46E-04	1.02E-02	1.23E-07	2.56E-04	2.14E+01	1.11E+00	1.39E-02	9.00E-02	5.16E-02
n-Butanol (C4H10O)	1	kg	2.22E+00	4.80E-03	3.87E-02	2.69E-07	4.31E-04	8.43E+01	2.59E+00	2.56E-02	1.67E-01	2.08E-01
chloroform (CHCl3)	1	kg	2.63E+00	3.99E-04	1.77E-02	1.25E-03	5.99E-04	3.72E+01	3.80E+00	1.80E-02	2.31E-01	8.60E-02
Indium (In)	1	kg	7.92E+02	2.23E-02	2.02E+00	1.23E-05	6.38E-01	2.66E+03	1.45E+02	2.93E+01	2.03E+01	1.42E+01
Tin (Sn)	1	kg	2.22E+01	2.60E-03	1.97E-01	1.51E-06	4.10E-03	3.34E+02	8.25E+00	2.49E-01	4.24E+00	2.43E+01

glass	1	kg	4.36E-01	6.68E-05	5.98E-03	7.39E-08	9.14E-05	1.29E+01	7.49E-01	9.49E-03	4.09E-02	3.36E-02
silica sand	1	kg	2.77E-02	7.14E-06	2.22E-04	2.37E-09	8.96E-06	4.43E-01	2.97E-02	6.70E-04	1.65E-03	1.01E-03
argon (Ar)	1	kg	1.76E+00	9.96E-05	1.09E-02	8.35E-08	3.54E-04	2.44E+01	1.26E+00	1.18E-02	1.67E-01	4.50E-02
oxygen (O2)	1	kg	6.68E-01	4.22E-05	4.60E-03	3.17E-08	1.15E-04	9.70E+00	5.36E-01	4.08E-03	8.04E-02	1.90E-02
nitrogen (N2)	1	kg	6.46E-01	4.09E-05	4.45E-03	3.07E-08	1.11E-04	9.39E+00	5.18E-01	1.20E-03	6.21E-02	1.82E-02
ethylene vinyl acetate	1	kg	1.41E+00	7.52E-04	3.43E-02	7.92E-08	1.95E-04	7.63E+01	1.97E+00	1.16E-02	8.37E-02	1.93E-01
aluminium (Al)	1	kg	4.43E+01	4.54E-03	4.44E-02	8.87E-07	3.79E-03	1.47E+02	4.99E-00	6.67E-02	4.01E-01	3.76E-01
Ilmenite	1	kg	3.43E-02	1.28E-05	1.14E-03	2.54E-08	1.24E-05	2.58E+00	3.27E-02	2.57E-04	2.84E-03	6.68E-03
Iron pellet/powder	1	kg	1.30E-01	2.21E-05	9.12E-04	1.43E-08	2.69E-05	1.81E+00	9.09E-02	1.29E-03	3.04E-02	5.44E-03
methane (CH4)	1	kg	1.28E+00	3.58E-04	6.56E-03	6.94E-08	1.18E-02	7.12E+01	8.14E-01	8.50E-01	1.09E-01	3.00E-02
Gold (Au)	1	kg	1.01E+06	2.54E+00	1.55E+02	9.73E-04	1.29E+01	1.18E+05	5.46E-03	1.88E+03	1.91E+04	2.84E+02
soda ash	1	kg	1.52E+00	1.03E-04	6.38E-03	7.20E-08	4.06E-04	1.39E+01	7.46E-01	1.13E-02	5.64E-02	3.39E-02
limestone	1	kg	1.82E-03	1.25E-06	1.92E-05	3.68E-10	9.07E-07	4.37E-02	2.29E-03	4.28E-05	6.74E-04	1.07E-04
dolomite	1	kg	3.81E-02	5.38E-06	2.64E-04	1.96E-09	8.92E-06	5.41E-01	3.26E-02	4.34E-04	4.34E-03	1.12E-03
cullet	1	kg	6.40E-02	2.31E-06	4.31E-05	1.02E-09	5.11E-06	9.43E-02	1.09E-02	2.32E-04	1.28E-03	2.19E-04
deionised water	1	kg	4.36E-03	1.76E-07	1.09E-05	7.95E-10	9.07E-07	2.41E-02	1.30E-03	2.09E-05	1.60E-04	4.82E-05
chlorine (Cl2)	1	kg	1.79E+00	9.74E-05	8.44E-03	1.20E-06	2.80E-04	1.80E+01	9.94E-01	1.25E-02	1.42E-01	3.71E-02
titanium dioxide (TiO2)	1	kg	2.69E+01	6.55E-03	4.50E-02	1.54E-06	1.70E-03	9.37E+01	6.44E+00	7.81E-02	5.76E-01	2.02E-01
isopropanol (C3H8O)	1	kg	1.03E+00	5.22E-03	2.78E-02	7.51E-08	1.49E-04	6.16E+01	1.69E+00	1.02E-02	5.40E-02	1.58E-01
acetone (C3H6O)	1	kg	1.36E-01	2.45E-04	3.07E-02	1.35E-09	5.73E-05	6.74E+01	2.07E+00	4.98E-03	2.86E-02	1.72E-01
acetic anhydride (C4H6O3)	1	kg	3.93E+00	1.58E-03	3.67E-02	4.71E-07	6.95E-04	7.88E+01	3.21E+00	3.82E-02	2.26E-01	1.91E-01
methylcyclohexane (C7H14)	1	kg	2.19E+00	2.21E-03	4.98E-02	1.70E-07	5.33E-04	1.06E+02	3.92E+00	4.21E-02	1.45E-01	2.66E-01
butyl acetate (C6H12O2)	1	kg	3.55E+00	5.68E-03	4.23E-02	4.16E-07	7.01E-04	9.20E+01	3.11E+00	4.01E-02	1.95E-01	2.25E-01
silver (Ag)	1	kg	1.70E+04	4.26E-02	2.60E+00	1.63E-05	2.17E-01	1.98E+03	9.17E+01	3.16E+01	3.21E+02	4.77E+00
adhesive	1	kg	4.14E-01	1.80E-04	1.18E-02	2.28E-07	1.49E-04	2.69E+01	3.71E-01	1.19E-02	2.40E-02	6.79E-02
dimethylformamide (C3H7NO)	1	kg	3.75E+00	9.53E-04	3.77E-02	4.65E-07	1.16E-03	8.04E+01	2.30E+00	2.85E-02	1.90E-01	2.03E-01
PET	1	kg	2.83E+00	5.25E-04	3.46E-02	1.31E-07	4.79E-04	7.62E+01	2.59E+00	3.15E-02	1.39E-01	1.88E-01
incineration of average residue	1	kg	7.48E+00	3.36E-05	1.25E-03	1.79E-08	1.05E-04	2.60E+00	3.93E-01	1.54E-02	4.85E-02	6.25E-03
inert material landfill	1	kg	2.88E-03	1.85E-06	7.33E-05	1.57E-09	1.07E-06	1.67E-01	4.50E-03	2.19E-04	2.51E-04	4.27E-04

3. Uncertainty sensitivity and Sensitivity analysis

Similar to the uncertainty analysis and sensitivity analyses for the TiO₂ module, those of the ZnO module are shown in Figure S6 and Figure S7, respectively.

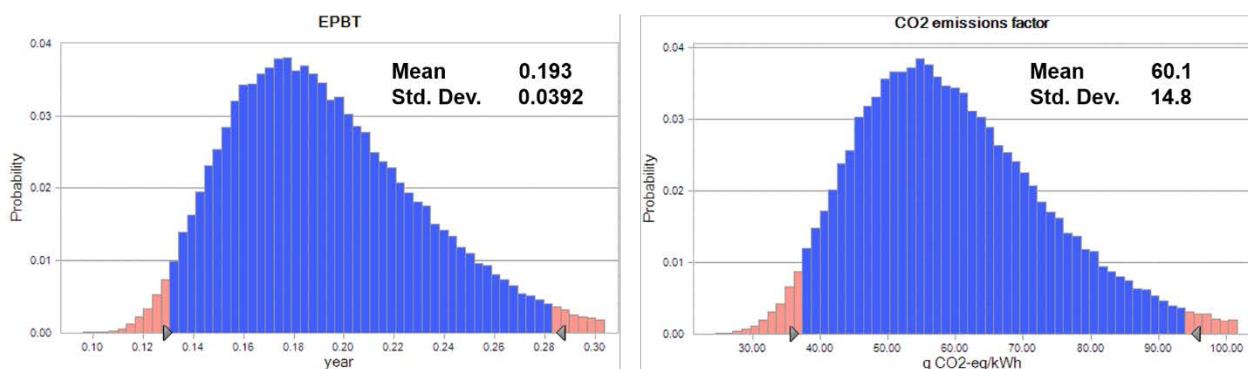


Figure S6. Probability distributions for energy payback time (EPBT) and CO₂ emissions factor of the ZnO Module.

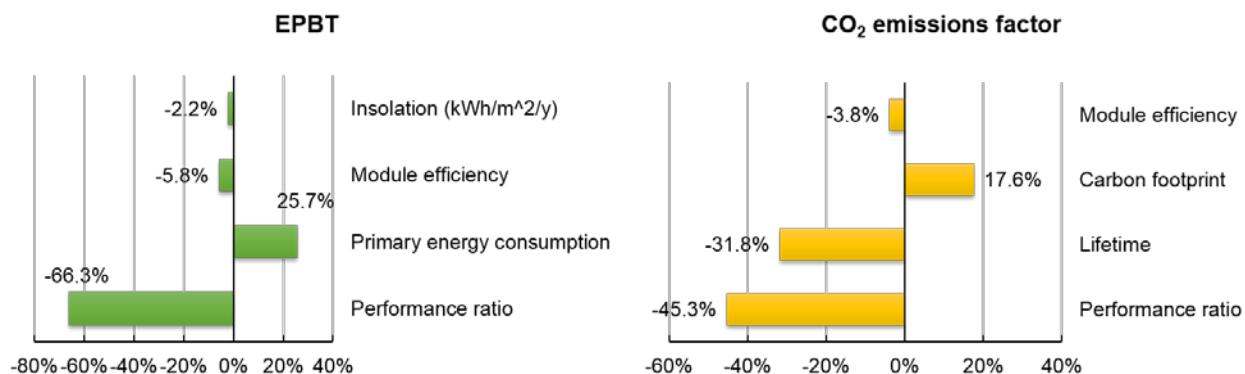


Figure S7. Sensitivity analysis for energy payback time (EPBT) and CO₂ emissions factor of the ZnO Module.

References

- Train, R.; Agee, T.; Gywin, A.; Martin, E. *Development Document for Interim Final Effluent Limitations. Guidelines and Proposed New Source Performance Standards for the significant inorganic products*; U.S. Environmental Protection Agency Washington, DC, 1975.
- Carr, D. S., Lead Compounds. In *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA: 2000.

3. Wang, L. K.; Shammas, N. K.; Hung, Y. T., *Biosolids Treatment Processes: Volume 6*. Humana Press: 2007.
4. Archive, R., Preparation of hydriodic acid (HI); <http://www.erowid.org/archive/rhodium/chemistry/hydriodic.html> (Last accessed December 2014).
5. G. S. Hiers, F. D. H., Anisole; <http://www.orgsyn.org/demo.aspx?prep=cv1p0058> (Last accessed December 2014).
6. S. Adimurthy, G. R., P. K. Ghosh, A. V. Bedekar, General procedure for the iodination; <https://www.erowid.org/archive/rhodium/chemistry/aromatic.iodination.iodide-iodate.html> (Last accessed December 2014).
7. Booth, G., Nitro Compounds, Aromatic. In *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA: 2000.
8. Coleman, G. H., Phenylhydrazine; <http://www.orgsyn.org/demo.aspx?prep=cv1p0442> (Last accessed December 2014).
9. Jianping Zou, R. Z., Tao Jiang, Shengyan Chen, A method for preparing 2-amino-biphenyl derivative. In Google Patents: 2014.
10. Schmidt, R.; Griesbaum, K.; Behr, A.; Biedenkapp, D.; Voges, H.-W.; Garbe, D.; Paetz, C.; Collin, G.; Mayer, D.; Höke, H., Hydrocarbons. In *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA: 2000.
11. Huiwen Shi, Z. B., Bin Shi, Zhenhua Zhang, Method for preparing coarse fluorene and fluorenone by taking wash oil as raw material. In Google Patents: 2012.
12. Yuan, W. Design and development of efficient solid-state dye-sensitized solar cells. Ph.D., Michigan State University, Ann Arbor, 2013.
13. Syrrakou, E.; Papaefthimiou, S.; Yianoulis, P., Environmental assessment of electrochromic glazing production. *Solar Energy Materials and Solar Cells* **2005**, 85, (2), 205-240.
14. Garcia-Valverde, R.; Cherni, J. A.; Urbina, A., Life cycle analysis of organic photovoltaic technologies. *Progress in Photovoltaics* **2010**, 18, (7), 535-558.
15. Kavan, L.; Gratzel, M., Highly Efficient Semiconducting TiO₂ Photoelectrodes Prepared by Aerosol Pyrolysis. *Electrochimica Acta* **1995**, 40, (5), 643-652.
16. Solaronix, Ti-Nanoxide T/SP; <http://shop.solaronix.com/titania-pastes/ti-nanoxide-t-sp.html> (Last accessed December 2014).
17. Liu, D. Y.; Kelly, T. L., Perovskite solar cells with a planar heterojunction structure prepared using room-temperature solution processing techniques. *Nature Photonics* **2014**, 8, (2), 133-138.
18. Supplies, S., SPI Silver Paste Plus(TM); http://www.2spi.com/catalog/spec_prep/plus_prop.html (Last accessed February, 2015).
19. Irizarry, R.; Yang, H. Process for making silver powder particles with small size crystallites. 2014.
20. Ecoinvent database v3.1; <http://www.ecoinvent.ch/> (Last accessed December 2014).