nature portfolio
https://doi.org/10.1038/s41893-021-00737-z

Supplementary information

Life cycle assessment of recycling strategies for perovskite photovoltaic modules

In the format provided by the authors and unedited

Life Cycle Assessment of Recycling Strategies for Perovskite Photovoltaic Modules

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This supplementary information file covers: (1) Material inventory and energy inventory for all the investigated modules; (2) Material inventory and energy inventory for recycling phase; (3) Life cycle impact assessment (LCIA) results for key raw materials; (4) LCIA results for other key components and the corresponding life cycle inventories (LCIs) retrieved from existing literature,[1,2] which are then converted by multiplying with updated characterization factors; (5) Lists of LCIA data extracted from Ecoinvent database;[3] (6) Environmental profiles of the metal oxide module, mixed-cation module, SnO_2 module, and semi-transparent module; (7) Primary energy consumption comparison between landfill and recycling end-of-life scenarios; (8) Comparison with existing PV technologies; (9) Uncertainty and sensitivity analysis results; (10) Impacts of recycling levels on the primary energy consumption and carbon footprint; (11) Levelized costs of electricity for PV systems based on recycled PV modules; (12) Sensitivity analysis results for recycling.

S1. Material inventory and energy inventory for all the investigated modules.

Supplementary Table 1. Material inventory of 1 m^2 of the LBSO module with an 80% active area.

	Mass (kg)	Notes
Substrate patterning		
FTO glass	5.040E+00	Substrate
Zinc power	7.130E-05	Chemical etching
Dilute HCl	1.868E-04	$Zn+2HCl \rightarrow ZnCl_2+H_2$
Ethanol	2.577E-02	Cleaning solvent
Deionized water	3.266E-02	Cleaning solvent
Acetone	1.470E-01	Cleaning solvent
BL deposition		
BL-TiO_2 ink	1.462E-02	70 nm of blocking layer
Ethanol	2.577E-02	Cleaning solvent

Deionized water	3.266E-02	Cleaning solvent
ETL deposition		
La-doped BSO NPs	1.158E-03	120 nm of ETL
2-Methoxyethanol	7.720E-04	Solvent of La-doped BSO NPs
Perovskite layer deposition		
PbI_2	1.156E-03	140 nm
Dimethylformamide	2.373E-03	Solvent of PbI_2
CH_3NH_3I	3.989E-04	300 nm
Isopropanol	3.126E-02	Solvent of CH_3NH_3I
Toluene	8.670E-04	Additive
HTL deposition		
PTAA solution	9.194E-03	HTL precursor
Cathode deposition		
Cu	1.434E-03	100 nm of electrode
Ar	1.081E-01	
O_2	1.081E-04	
Direct emissions		
$ZnCl_2$	1.044E-04	Resultants from chemical etching
H_2	1.536E-06	Resultants from chemical etching
Ethanol	1.328E-02	Solvent in BL-TiO_2 ink
$TiCl_4$	1.406E-04	Wasted effective component of BL-TiO_2 ink
Isopropanol	3.215E-02	Solvent in BL-TiO_2 ink and solvent of CH_3NH_3I
Acetone	4.298E-04	Solvent in BL-TiO_2 ink
Acetic anhydride	7.573E-04	Solvent in BL-TiO_2 ink
La-doped BSO NPs	8.109E-04	Wasted effective component of LBSO ink
2-Methoxyethanol	7.720E-04	Solvent in LBSO ink
PbI_2	8.095E-04	Wasted PbI_2
Dimethylformamide	2.373E-03	Solvent of PbI_2

CH_3NH_3I	2.793E-04	Wasted CH_3NH_3I
PTAA	1.050E-05	Wasted effective component of PTAA solution
LiTFSI	1.190E-04	Wasted effective component of PTAA solution
Toluene	2.168E-03	Solvent in PTAA solution and waste from spin coating
Acetonitrile	7.860E-04	Solvent in PTAA solution
4-tert-butylpyridine	6.923E-03	Solvent in PTAA solution
Cu	7.168E-04	Wasted copper
Ar	1.081E-01	
O_2	1.081E-04	
Mass of module	**5.041**	Landfill

Supplementary Table 2. Energy inventory of 1 m^2 of the LBSO module with an 80% active area.

	Power (W)	Time (s)	Electricity (kWh)
Substrate patterning			
Sonication	1.200E+04	1,200	4.00
BL deposition			
Spray pyrolysis	1.300E+02	19	6.69E-04
ETL deposition			
LBSO spin coating	3.860E+05	30	3.22
Calcining	7.200E+04	3,600	72.0
Perovskite layer deposition			
1^{st}-step spin coating	4.289E+04	10	0.119
2^{nd}-step spin coating	1.072E+06	20	5.96
Drying	1.440E+04	600	2.40
HTL deposition			

PTAA spin coating	3.860E+05	30	3.22
Electrode deposition			
Sputtering	7.150E+04	182	7.78
Total			**98.7**

Supplementary Table 3. Material inventory of 1 m^2 of the defect-engineered module with an 80% active area.

	Mass (kg)	Notes
Substrate		
FTO glass	5.040E+00	Substrate
BL deposition		
BL-TiO_2 ink	1.253E-02	60 nm of blocking layer
ETL deposition		
MP-TiO_2	5.076E-04	150 nm of ETL
2-Methoxyethanol	2.449E-03	Solvent of MP-TiO_2
Isopropanol	2.577E-02	
Perovskite layer deposition		
PbI_2	7.672E-04	156 nm
$PbBr_2$	1.566E-05	3 nm
FAI	2.463E-04	286 nm
MABr	3.079E-05	55 nm
Dimethylformamide	9.709E-03	Solvent
DMSO	2.816E-04	Solvent
Isopropanol	2.420E-03	Solvent
HTL deposition		
PTAA solution	8.909E-04	HTL precursor
Isopropanol	2.577E-02	

Cathode deposition		
Cu	1.434E-03	100 nm of electrode
Ar	1.081E-01	
O_2	1.081E-04	
Encapsulation		
Adhesive	2.020E-02	
PET	6.170E-02	
Direct emissions		
$TiCl_4$	1.206E-04	Wasted effective component of BL-TiO_2 ink
Isopropanol	3.182E-03	Solvent
Acetone	3.684E-04	Solvent
Acetic anhydride	6.491E-04	Solvent
2-Methoxyethanol	2.449E-03	Solvent in MP-TiO_2 ink
Dimethylformamide	9.709E-04	Solvent
DMSO	2.816E-04	Solvent
Toluene	8.700E-04	Solvent in PTAA solution
Acetonitrile	5.895E-06	Solvent in PTAA solution
Cu	7.168E-04	
Ar	1.081E-01	
O_2	1.081E-04	
Mass of module	**5.135**	Landfill

Supplementary Table 4. Energy inventory of 1 m^2 of the defect-engineered module with an 80% active area.

	Power (W)	Time (s)	Electricity (kWh)
BL deposition			
Spray pyrolysis	1.300E+02	16	5.74E-04

ETL deposition			
MP-TiO_2 slot-die coating	2.500E+03	30	0.0208
Calcining	4.286E+04	3,600	42.9
Perovskite layer deposition			
1st-step slot-die coating	2.500E+03	43	0.0298
2nd-step slot-die coating	2.500E+03	43	0.0298
1st-step drying	8.571E+03	1,800	4.29
2nd-step drying	1.286E+04	1,800	6.43
Annealing	8.571E+03	1,800	4.29
HTL deposition			
PTAA slot-die coating	2.500E+03	200	0.139
Electrode deposition			
Sputtering	7.150E+04	182	7.78
Encapsulation			
Lamination	1.500E+03	30	0.0125
Total			**65.9**

Supplementary Table 5. Material inventory of 1 m^2 of the metal oxide module with an 80% active area.[4]

	Mass (kg)	Notes
Substrate patterning		
ITO glass	1.540E+00	Substrate
Ethanol	2.577E-02	Cleaning solvent
Deionized water	3.266E-02	Cleaning solvent
HTL deposition		
$Ni(NO_3)_2 \cdot 6H_2O$	2.831E-03	80 nm of HTL
Ethylene glycol	8.281E-03	Solvent of $Ni(NO_3)_2 \cdot 6H_2O$
Ethylenediamine	2.047E-03	Solvent of $Ni(NO_3)_2 \cdot 6H_2O$
Perovskite layer deposition		
PbI_2	8.410E-04	102 nm
Dimethylformamide	1.733E-03	Solvent of PbI_2

CH_3NH_3I	2.901E-04	218 nm
Isopropanol	4.555E-03	Solvent of CH_3NH_3I
ETL deposition		
ZnO powder	5.236E-04	70 nm of ETL
Chlorobenzene	2.566E-02	Solvent of ZnO, concentration 2%
Cathode deposition		
Al	2.634E-04	70 nm of electrode
Direct emissions		
$Ni(NO_3)_2·6H_2O$	1.982E-03	Wasted effective component of NiO_x ink
Ethylene glycol	8.281E-03	Solvent in NiO_x ink
Ethylenediamine	2.047E-03	Solvent in NiO_x ink
PbI_2	5.887E-04	Wasted PbI_2
Dimethylformamide	1.733E-03	Solvent of PbI_2
CH_3NH_3I	2.031E-04	Wasted CH_3NH_3I
Isopropanol	4.555E-03	Solvent of CH_3NH_3I
ZnO powder	3.665E-04	Wasted effective component of ZnO ink
Chlorobenzene	2.566E-02	Solvent in ZnO ink
Al	4.741E-05	Wasted aluminum
Nitrogen	3.483E+00	
Mass of module	**1.542**	Landfill

Supplementary Table 6. Energy inventory of 1 m^2 of the metal oxide module with an 80% active area.[4]

	Power (W)	Time (s)	Electricity (kWh)
Substrate patterning			
Sonication	1.200E+04	1,200	4.00
HTL deposition			
NiO_x spin coating	2.681E+05	90	6.70
Post-annealing	4.320E+04	3,600	43.2
Perovskite layer deposition			
Nitrogen glove box	3.000E+04	630	5.25
1^{st}-step spin coating	4.289E+04	10	0.119
Drying	1.008E+04	600	1.68
2^{nd}-step spin coating	1.072E+06	20	5.96
Annealing	1.440E+04	7,200	28.8
ETL deposition			

ZnO spin coating	2.681E+05	90	6.70
Electrode deposition			
Vacuum pump	3.680E+04	900	9.20
Evaporation	3.840E+04	500	5.33
Cooling	1.600E+04	3,600	16.0
Total			**133**

Supplementary Table 7. Material inventory of 1 m^2 of the mixed-cation module with an 80% active area.[5]

	Mass (kg)	Notes
Substrate patterning		
FTO glass	5.040E+00	Substrate
Ethanol	2.577E-02	Cleaning solvent
Acetone	1.470E-01	Cleaning solvent
BL deposition		
BL-TiO_2 ink	6.266E-03	30 nm of blocking layer
Ethanol	2.577E-02	Cleaning solvent
Deionized water	3.266E-02	Cleaning solvent
ETL deposition		
TiO_2	1.128E-03	200 nm of ETL
Ethanol	2.051E-04	Solvent of TiO_2 paste
Perovskite layer deposition		
FAI	4.118E-04	287 nm of FAI
PbI_2	1.159E-03	141 nm of PbI_2
MABr	4.969E-05	53 nm of MABr
$PbBr_2$	1.628E-04	18 nm of $PbBr_2$
DMF	1.644E-03	Solvent of mixed-cation mixtures
DMSO	4.789E-04	Solvent of mixed-cation mixtures
Chlorobenzene	1.221E-04	Additive
HTL deposition		
Spiro-OMeTAD	4.853E-04	200 nm of HTL
HTFSI	5.683E-05	Additive
Acetonitrile	2.628E-04	Solvent of HTFSI
FK209	1.786E-05	Additive
4-tert-Butylpyridine	1.782E-04	Additive
Chlorobenzene	7.327E-03	Solvent of Spiro-OMeTAD

Cathode deposition		
Cu	1.147E-03	80 nm of electrode
Ar	8.650E-02	
O_2	8.650E-05	
Direct emissions		
Ethanol	5.894E-03	Solvent of BL-TiO_2 ink and TiO_2 paste
$TiCl_4$	6.028E-05	Wasted effective component of BL-TiO_2 ink
Isopropanol	3.810E-04	Solvent of BL-TiO_2 ink
Acetone	1.842E-04	Solvent of BL-TiO_2 ink
Acetic anhydride	3.246E-04	Solvent of BL-TiO_2 ink
TiO_2	7.896E-04	Wasted TiO_2 paste
FAI	2.883E-04	Wasted FAI
PbI_2	8.113E-04	Wasted PbI_2
MABr	3.478E-05	Wasted MABr
$PbBr_2$	1.140E-04	Wasted $PbBr_2$
DMF	1.644E-03	Solvent of mixed-cation mixtures
DMSO	4.789E-04	Solvent of mixed-cation mixtures
Chlorobenzene	7.449E-03	Solvent of Spiro-OMeTAD and waste from spin coating
Spiro-OMeTAD	3.397E-04	Wasted Spiro-OMeTAD
HTFSI	3.978E-05	Wasted Li-TFSI
Acetonitrile	2.628E-04	Solvent of HTFSI
FK209	1.250E-05	Wasted FK209
4-tert-Butylpyridine	1.247E-04	Wasted 4-tert-Butylpyridine
Cu	5.734E-04	Wasted copper
Ar	8.650E-02	
O_2	8.650E-05	
Mass of module	**5.041**	Landfill

Supplementary Table 8. Energy inventory of 1 m^2 of the mixed-cation module with an 80% active area.[5]

	Power (W)	Time (s)	Electricity (kWh)
Substrate patterning			
Sonication	1.200E+04	1,200	4.00
BL deposition			
Spray pyrolysis	1.300E+02	8	2.87E-04

ETL deposition			
MP-TiO_2 spin coating	7.422E+05	15	3.09
Calcining	7.200E+04	1,200	24.0
Perovskite layer deposition			
1st-step spin coating	4.289E+04	10	0.119
2nd-step spin coating	1.393E+06	30	11.6
Drying	1.440E+04	5,400	21.6
HTL deposition			
Spiro-OMeTAD spin coating	3.860E+05	20	2.14
Electrode deposition			
Sputtering	7.150E+04	145	7.06
Total			**73.6**

Supplementary Table 9. Material inventory of 1 m^2 of the SnO_2 module with an 80% active area.[6]

	Mass (kg)	Notes
Substrate		
ITO glass	1.540E+00	Substrate
ETL deposition		
SnO_2	1.390E-04	25 nm of HTL
H_2O	5.067E-03	Solvent
Isopropanol	2.577E-02	
Perovskite layer deposition		
PbI_2	1.105E-03	224 nm
Dimethylformamide	1.660E-03	Solvent
DMSO	1.014E-04	Solvent
FAI	2.927E-04	340 nm
MABr	2.927E-05	52 nm
MACl	2.927E-05	33 nm
Isopropanol	3.834E-03	Solvent
HTL deposition		
Spiro-OMeTAD	2.621E-04	180 nm of HTL
LiTFSI	3.299E-05	Additive
acetonitrile	9.972E-05	
4-tert butylpyridine	1.004E-04	
chlorobenzene	4.024E-03	Solvent

Isopropanol	2.577E-02	
Cathode deposition		
Cu	8.602E-04	60 nm of electrode
Ar	6.487E-02	
O_2	6.487E-05	
Encapsulation		
Adhesive	2.020E-02	
PET	6.170E-02	
Direct emissions		
H_2O	5.067E-03	
DMF	1.660E-03	
DMSO	1.014E-04	
IPA	3.834E-03	
acetonitrile	9.972E-05	
chlorobenzene	4.024E-03	
Cu	4.301E-04	
Ar	6.487E-02	
O_2	6.487E-05	
Mass of module	**1.624**	Landfill

Supplementary Table 10. Energy inventory of 1 m^2 of the SnO_2 module with an 80% active area.[6]

	Power (W)	Time (s)	Electricity (kWh)
Substrate treatment			
UV/O_3 cleaning	1.380E+02	600	0.0230
ETL deposition			
SnO_2 slot-die coating	2.500E+03	30	0.0208
Annealing	1.286E+04	1,800	6.43
Perovskite layer deposition			
1^{st}-step slot-die coating	2.500E+03	43	0.0298
Annealing	6.000E+03	60	0.100
2^{nd}-step slot-die coating	2.500E+03	43	0.0298
Post-annealing	1.286E+04	900	3.21
HTL deposition			
Spiro-OMeTAD slot-die coating	2.500E+03	200	0.139
Electrode deposition			

Sputtering	7.150E+04	109	6.33
Encapsulation			
Lamination	1.500E+03	30	0.0125
Total			**16.3**

Supplementary Table 11. Material inventory of 1 m^2 of the semi-transparent module with an 80% active area.[7]

	Mass (kg)	Notes
Substrate		
ITO glass	1.540E+00	Substrate
HTL deposition		
Ni	6.344E-04	70 nm of HTL
Ar	7.568E-02	
O_2	2.100E-04	
PL deposition		
PbI_2	8.242E-04	100 nm
DMF	1.945E-03	Solvent
MAI	2.529E-04	190 nm
MACl	1.331E-05	10 nm
Ethanol	4.201E-03	Solvent
Nitrogen	1.825E+00	Inert gas purging
ETL deposition		
PCBM	1.000E-04	50 nm
Al_2O_3	1.116E-05	50 nm of AZO
ZnO	3.595E-04	
Electrode deposition		
ITO	3.084E-03	270 nm of electrode
Ar	2.919E-01	
O_2	2.919E-04	
Direct emissions		
NiO	4.047E-04	
PbI_2	3.297E-04	
DMF	1.945E-03	
MAI	1.012E-04	
MACl	5.324E-06	
Ethanol	4.201E-03	

PCBM	4.000E-05	
AZO	1.483E-04	
Ar	3.676E-01	
O_2	3.269E-04	
Nitrogen	1.825E+00	
Mass of module	**1.544**	Landfill

Supplementary Table 12. Energy inventory of 1 m^2 of the semi-transparent module with an 80% active area.[7]

	Power (W)	Time (s)	Electricity (kWh)
Substrate treatment			
UV/O_3 cleaning	1.380E+02	1,200	0.0460
HTL deposition			
Sputtering	9.017E+04	127	7.35
Perovskite layer deposition			
Nitrogen glove box	3.000E+04	330	2.75
PbI_2 spin coating	3.860E+05	90	9.65
MAI/MACl spin coating	6.862E+05	90	17.2
MACl treatment	1.440E+04	60	0.240
ETL deposition			
PCBM spin coating	2.102E+04	60	0.350
AZO layer spin coating	4.289E+04	30	0.357
Electrode deposition			
Sputtering	7.990E+04	491	10.9
Total			**48.8**

S2. Material inventory and energy inventory for recycling phase

Supplementary Table 13. Material inventory of recycling 1 m^2 of the module with FTO substrate.

	Mass (kg)	Notes
The LBSO module		
DMF	1.264E+00	Solvent for selective dissolution
Deionized water	3.280E-02	Cleaning solvent
The mixed-cation module		

DMF	1.264E+00	Solvent for selective dissolution
Deionized water	3.277E-02	Cleaning solvent

Supplementary Table 14. Energy inventory of recycling 1 m^2 of the module with FTO substrate.

	Power (W)	Time (s)	Electricity (kWh)
The LBSO module			
Annealing at 500 °C	3.409E+03	3,600	3.41
The mixed-cation module			
Annealing at 500 °C	3.409E+03	3,600	3.41

Supplementary Table 15. Material inventory of recycling 1 m^2 of the module with ITO substrate.

	Mass (kg)	Notes
The metal oxide module		
NaOH (50%)	6.902E-04	Solvent for aqueous base
Deionized water	4.307E-01	Diluent

Supplementary Table 16. Energy inventory of recycling 1 m^2 of the module with ITO substrate.

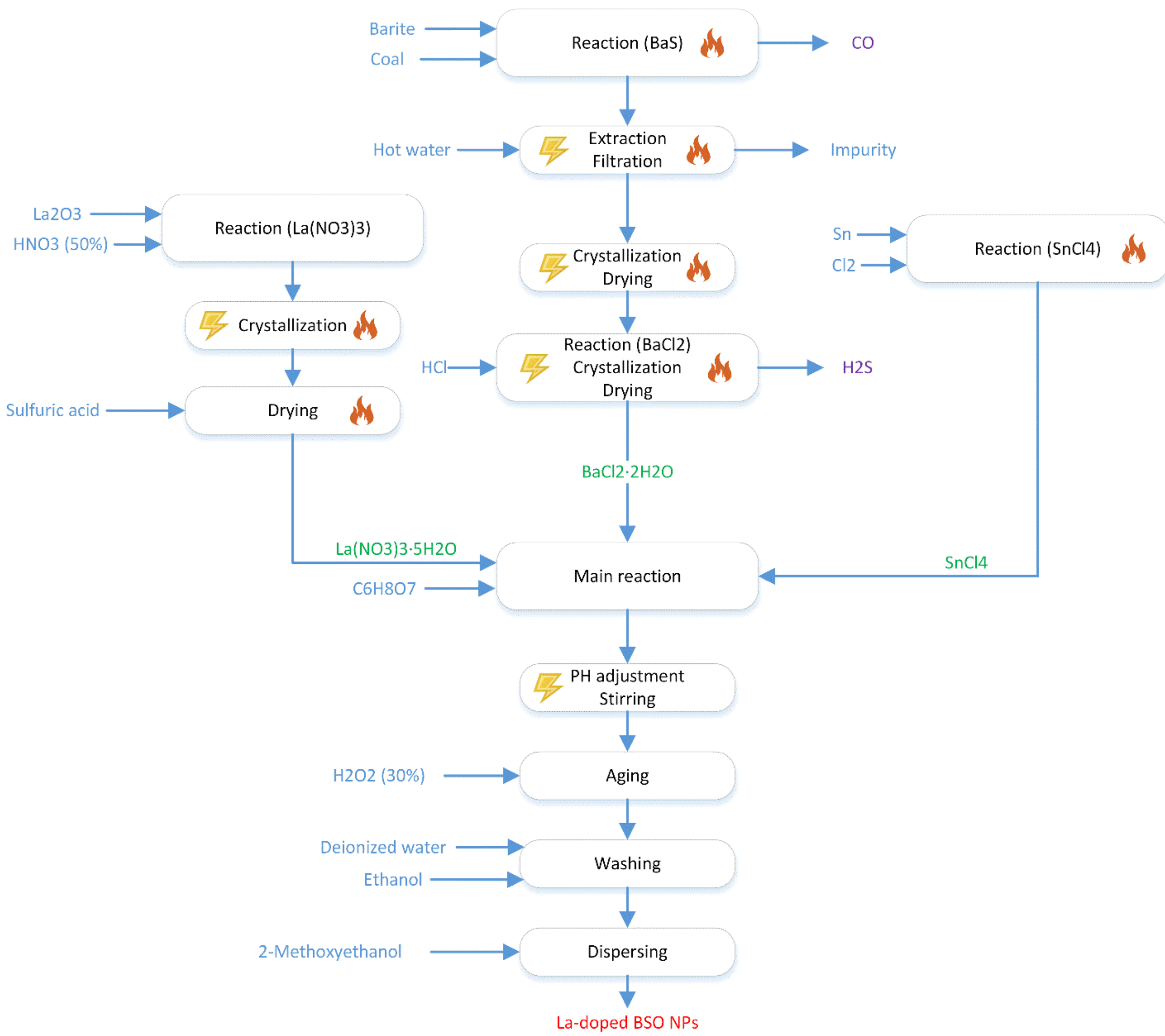
	Power (W)	Time (s)	Electricity (kWh)
The metal oxide module			
Ultrasonic cleaning	8.810E+02	900	0.220

S3. LCIA results for key raw materials

In this section, blue inflows in the charts represent raw materials, items in green refer to intermediate products, purple outflows represent by-products, and outflows in red represent the target products. The flame symbols in the box mean that heating utility is needed in the procedures, the lightning suggests the procedures consume electricity, and snowflake represents that cooling utility is required in the corresponding steps. In order to accurately reveal the individual contribution of target product to the overall environmental impacts of the studied system, mass-based allocation method is employed, which is frequently used in recent life cycle assessment (LCA) studies.[8]

S3.1 LBSO nanoparticle solution

Supplementary Figure 1 shows the manufacturing route of LBSO nanoparticle solution, which is based on the description of Shin et al.[9] The LCI and the corresponding LCIA results of 1 kg of LBSO nanoparticle solution are available in Supplementary Table 17 and Supplementary Table 18, respectively. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.



Supplementary Figure 1. Manufacturing route for LBSO nanoparticle solution.

Supplementary Table 17. LCI for 1 kg of LBSO nanoparticle solution.

	Value	Unit

Process input		
$C_6H_8O_7$	3.431E-01	kg
H_2O_2 (50%)	4.020E-02	kg
2-Methoxyethanol	6.664E-01	kg
H_2O	1.169E+00	kg
La_2O_3	2.922E-02	kg
HNO_3 (50%)	6.776E-02	kg
Barite	8.791E-01	kg
Coal	2.264E-01	kg
HCl	8.263E-01	kg
Sn	4.253E-01	kg
Cl_2	5.076E-01	kg
heat	7.880E+00	MJ
electricity	1.125E-01	kWh
Process output		
$Ba_{0.95}La_{0.05}SnO_3$	1.000E+00	kg
2-Methoxyethanol	6.664E-01	kg
CO	3.803E-01	kg
H_2S	1.155E-01	kg
wastewater	1.556E+00	kg
waste	1.462E+00	kg

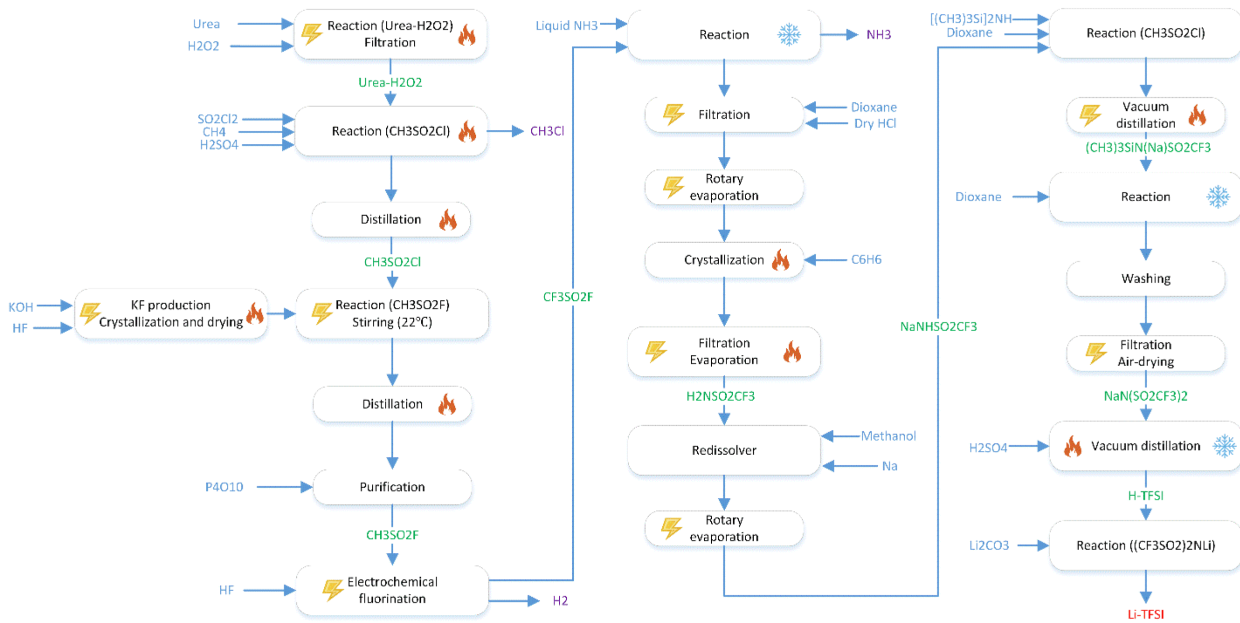
Supplementary Table 18. LCIA results for 1 kg of LBSO nanoparticle solution.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	7.712E+00
Cumulative energy demand (MJ-Eq)	1.242E+02
Agricultural land occupation (m^2a)	1.572E+00
Climate change (kg CO_2-Eq)	6.925E+00
Fossil depletion (kg oil-Eq)	2.285E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	1.662E-01
Freshwater eutrophication (kg P-Eq)	4.205E-03

Human toxicity (kg 1,4-DCB-Eq)	1.885E+02
Ionising radiation (kg U235-Eq)	6.452E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.515E+02
Marine eutrophication (kg N-Eq)	1.584E-02
Metal depletion (kg Fe-Eq)	2.928E+02
Natural land transformation (m^2)	1.743E-02
Ozone depletion (kg CFC-11-Eq)	7.642E-07
Particulate matter formation (kg PM10-Eq)	7.226E-02
Photochemical oxidant formation (kg NMVOC)	5.003E-02
Terrestrial acidification (kg SO_2-Eq)	1.108E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	6.143E-03
Urban land occupation (m^2a)	3.059E-01
Water depletion (m^3)	8.075E-02
Ecosystem quality (points)	1.649E+00
Human health (points)	1.706E+00
Resources (points)	1.387E+01

S3.2 LiTFSI

Supplementary Figure 2 shows the complete manufacturing route of Lithium bis (trifluoromethylsulphonyl) imide (LiTFSI). Methanesulfonyl chloride (MSC) is synthesized from methane and sulfuryl chloride following Sudip Mukhopadhyay's method.[10] The synthesis method of Bis ((trifluoromethyl) sulfonyl) imide (HTFSI) is extracted from existing literature.[11] HTFSI is then converted to the desired salt (LiTFSI) via neutralizing with lithium carbonate.[12] The LCI and the corresponding LCIA results of 1 kg of LiTFSI are shown in Supplementary Table 19 and Supplementary Table 20. Note that water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.



Supplementary Figure 2. Manufacturing route for LiTFSI.

Supplementary Table 19. LCI for 1 kg of LiTFSI.

	Value	Unit
Process input		
H_2O	2.879E+00	kg
methanol	2.546E+00	kg
Li_2CO_3	1.289E-01	kg
H_2SO_4	7.267E+01	kg
dioxane	8.959E+00	kg
$[(CH_3)_3Si]_2NH$	4.761E+00	kg
Na	1.266E-01	kg
SO_2Cl_2	1.283E+01	kg
CH_4	3.961E+01	kg
urea	3.148E-01	kg
H_2O_2	3.568E-01	kg
KOH	1.624E+00	kg
HF	1.283E+00	kg
liquid NH_3	3.747E+00	kg

dry HCl	2.011E-01	kg
C_6H_6	1.563E+00	kg
cooling	1.250E+00	MJ
heat	2.922E+01	MJ
electricity	2.851E+02	kWh
Process output		
$(CF_3SO_2)_2NLi$	1.000E+00	kg
H_2	7.028E-02	kg
CH_3Cl	7.102E+00	kg
NH_3	3.466E+00	kg
CO_2	7.666E-02	kg
wastewater	4.600E+00	kg
waste	1.373E+02	kg

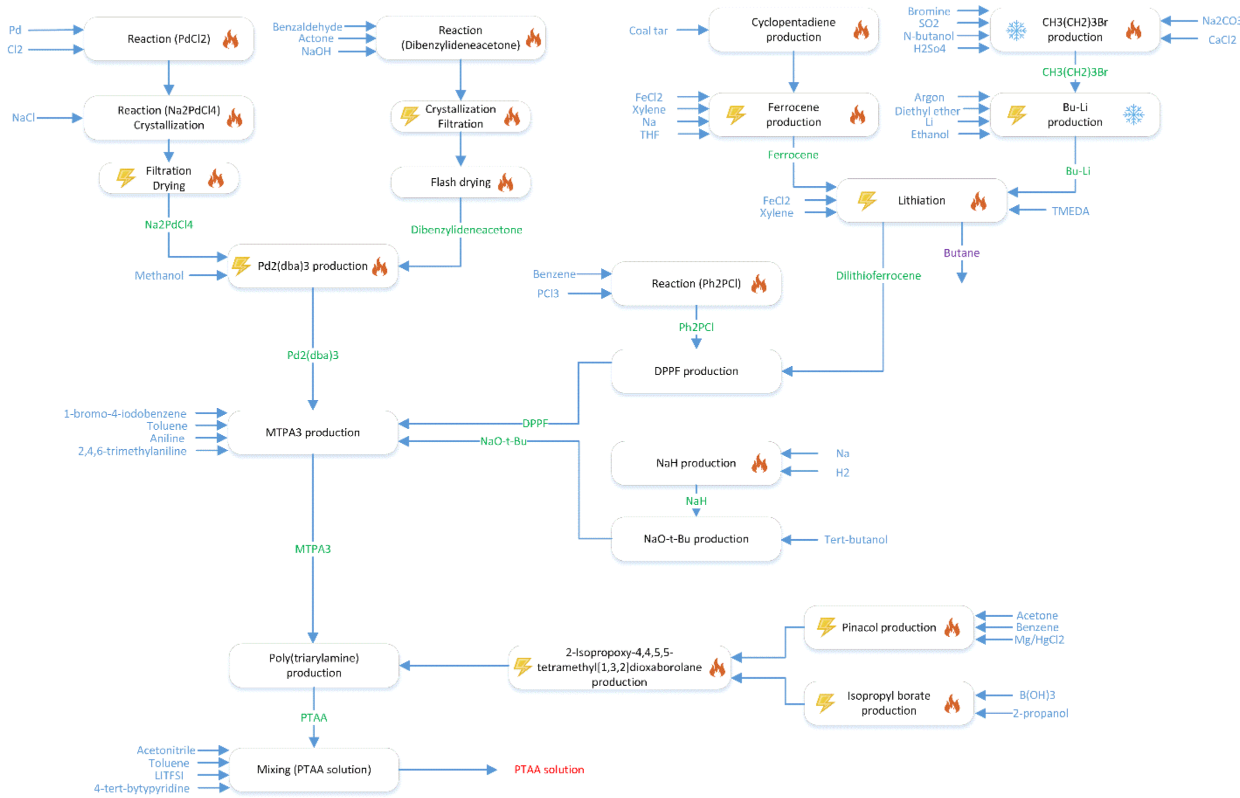
Supplementary Table 20. LCIA results for 1 kg of LiTFSI.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	4.441E+01
Cumulative energy demand (MJ-Eq)	6.967E+02
Agricultural land occupation (m^2a)	3.681E+00
Climate change (kg CO_2-Eq)	3.771E+01
Fossil depletion (kg oil-Eq)	1.497E+01
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	2.171E+00
Freshwater eutrophication (kg P-Eq)	4.137E-02
Human toxicity (kg 1,4-DCB-Eq)	1.860E+03
Ionising radiation (kg U235-Eq)	2.025E+00
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.529E+03
Marine eutrophication (kg N-Eq)	4.527E-02
Metal depletion (kg Fe-Eq)	1.353E+00
Natural land transformation (m^2)	6.327E-03
Ozone depletion (kg CFC-11-Eq)	5.283E-06
Particulate matter formation (kg PM10-Eq)	9.033E-02

Photochemical oxidant formation (kg NMVOC)	1.323E-01
Terrestrial acidification (kg SO_2-Eq)	2.842E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	3.511E-02
Urban land occupation (m^2a)	3.567E-01
Water depletion (m^3)	9.077E-02
Ecosystem quality (points)	1.767E+00
Human health (points)	1.425E+01
Resources (points)	1.858E+00

S3.3 PTAA solution

Supplementary Figure 3 demonstrates the manufacturing route of Poly(bis(4-phenyl)(2,4,6-trimethylphenyl)amine) (PTAA) solution. PTAA is synthesized via Suzuki coupling according to the description in the literature.[13] N,N-bis(4-bromophenyl)-2,4,6-trimethylaniline (MTPA3) is one of the key precursors for PTAA production, whose synthesis mechanism is found in a doctoral dissertation.[14] The manufacturing processes of Dibenzylideneacetone,[15] $Pd_2(dba)_3$,[16] DPPF,[17] NaH,[18] and Isopropyl borate,[19] are retrieved from existing publications. Finally, the PTAA solution is prepared by mixing 5 different reagents which is detailed by Shin et al.[9] The LCI and the corresponding LCIA results of 1 kg of PTAA solution are listed in Supplementary Table 21 and Supplementary Table 22. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.



Supplementary Figure 3. Manufacturing route for PTAA solution.

Supplementary Table 21. LCI for 1 kg of PTAA solution.

	Value	Unit
Process input		
Benzaldehyde	9.234E-05	kg
NaOH (50%)	1.835E-04	kg
NaCl	3.058E-05	kg
Pd	2.770E-05	kg
Cl_2	1.856E-05	kg
xylene	5.175E-04	kg
tetrahydrofuran	5.349E-04	kg
$FeCl_2$	9.514E-05	kg
coal tar	3.971E-04	kg
hexanes	1.546E-03	kg
Ar	2.266E-06	kg

diethyl ether	5.429E-04	kg
bromine	1.336E-04	kg
sulfur dioxide	5.343E-05	kg
n-butanol	9.884E-05	kg
sodium carbonate	5.566E-06	kg
calcium chloride	1.670E-06	kg
Li	2.183E-05	kg
ethanol	2.103E-04	kg
TMEDA	6.589E-05	kg
PCl_3	1.220E-04	kg
1-bromo-4-iodobenzene	1.117E-02	kg
tert-butanol	3.493E-03	kg
H_2	4.720E-05	kg
aniline	1.749E-03	kg
ethyl acetate	7.712E-02	kg
EDTA	3.676E-02	kg
2,4,6-trimethylaniline	2.539E-03	kg
Trimethyl borate	7.578E-03	kg
Isopropyl alcohol	3.552E-03	kg
Mg	2.189E-04	kg
acetone	1.667E-03	kg
Hg	1.820E-04	kg
HNO_3 (50%)	1.141E-04	kg
HCl (30%)	2.203E-04	kg
N_2	2.435E-05	kg
toluene	1.711E-01	kg
H_2O	1.528E-01	kg
methanol	5.318E-02	kg
Li_2CO_3	2.384E-03	kg
H_2SO_4	1.344E+00	kg
dioxane	1.657E-01	kg

$[(CH_3)_3Si]_2NH$	8.804E-02	kg
Na	3.461E-03	kg
SO_2Cl_2	2.372E-01	kg
CH_4	7.325E-01	kg
urea	5.821E-03	kg
H_2O_2	6.597E-03	kg
KOH	3.002E-02	kg
HF	2.372E-02	kg
liquid NH_3	6.929E-02	kg
dry HCl	3.718E-03	kg
C_6H_6	3.276E-02	kg
acetonitrile	8.549E-02	kg
4-tert-butylpyridine	7.529E-01	kg
cooling	2.322E-02	MJ
heat	6.848E-01	MJ
electricity	1.371E+01	kWh
Process output		
PTAA solution	1.000E+00	kg
H_2	1.299E-03	kg
CH_3Cl	1.313E-01	kg
NH_3	6.419E-02	kg
CO_2	1.417E-03	kg
C_3H_8O	8.530E-04	kg
azeotrope	4.311E-03	kg
$Mg(OH)_2$	2.457E-04	kg
butane	5.095E-05	kg
N_2	2.435E-05	kg
Ar	2.266E-06	kg
NO_2	4.164E-05	kg
wastewater	1.847E-01	kg
waste	2.723E+00	kg

Supplementary Table 22. LCIA results for 1 kg of PTAA solution.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	2.113E+01
Cumulative energy demand (MJ-Eq)	3.576E+02
Agricultural land occupation (m^2a)	1.140E+00
Climate change (kg CO_2-Eq)	1.892E+01
Fossil depletion (kg oil-Eq)	7.781E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	5.382E-01
Freshwater eutrophication (kg P-Eq)	1.111E-02
Human toxicity (kg 1,4-DCB-Eq)	5.676E+02
Ionising radiation (kg U235-Eq)	1.026E+00
Marine ecotoxicity (kg 1,4-DCB-Eq)	4.281E+02
Marine eutrophication (kg N-Eq)	2.253E-02
Metal depletion (kg Fe-Eq)	1.316E+00
Natural land transformation (m^2)	2.969E-03
Ozone depletion (kg CFC-11-Eq)	3.218E-06
Particulate matter formation (kg PM10-Eq)	5.734E-02
Photochemical oxidant formation (kg NMVOC)	6.765E-02
Terrestrial acidification (kg SO_2-Eq)	1.871E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	5.573E-02
Urban land occupation (m^2a)	1.322E-01
Water depletion (m^3)	4.260E-02
Ecosystem quality (points)	8.024E-01
Human health (points)	4.672E+00
Resources (points)	9.903E-01

S3.4 NiO_x precursor solution

The NiO_x precursor solution is prepared according to the technical details in a paper by You et al.[4]

Supplementary Table 23 and Supplementary Table 24 exhibit the LCI and the corresponding LCIA results of 1 kg of NiO_x precursor solution. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.

Supplementary Table 23. LCI for 1 kg of NiO_x precursor solution.

	Value	Unit
Process input		
ethylene glycol	6.293E-01	kg
ethylenediamine	1.555E-01	kg
HNO_3 (50%)	1.863E-01	kg
$NiSO_4$	1.146E-01	kg
KOH	8.280E-02	kg
H_2O	1.303E+00	kg
heat	6.197E+00	MJ
electricity	5.077E-03	kWh
Process output		
NiO_x precursor solution	1.000E+00	kg
K_2SO_4	1.286E-01	kg
wastewater	1.343E+00	kg

Supplementary Table 24. LCIA results for 1 kg of NiO_x precursor solution.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	3.266E+00
Cumulative energy demand (MJ-Eq)	6.471E+01
Agricultural land occupation (m^2a)	7.461E-01
Climate change (kg CO_2-Eq)	2.847E+00
Fossil depletion (kg oil-Eq)	1.259E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	1.177E-01
Freshwater eutrophication (kg P-Eq)	2.210E-03
Human toxicity (kg 1,4-DCB-Eq)	1.383E+02
Ionising radiation (kg U235-Eq)	2.423E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.363E+02
Marine eutrophication (kg N-Eq)	5.890E-03
Metal depletion (kg Fe-Eq)	1.677E+00

Natural land transformation (m^2)	3.903E-04
Ozone depletion (kg CFC-11-Eq)	4.301E-07
Particulate matter formation (kg PM10-Eq)	2.891E-02
Photochemical oxidant formation (kg NMVOC)	2.067E-02
Terrestrial acidification (kg SO_2-Eq)	1.172E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	9.879E-03
Urban land occupation (m^2a)	3.762E-02
Water depletion (m^3)	1.619E-02
Ecosystem quality (points)	1.751E-01
Human health (points)	1.113E+00
Resources (points)	2.207E-01

S3.5 ZnO precursor solution

We derive the manufacturing procedure following the method of You et al.[4] The LCI and the corresponding LCIA results of 1 kg of NiO_x precursor solution are demonstrated in

Supplementary Table 25 and Supplementary Table 26. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.

Supplementary Table 25. LCI for 1 kg of ZnO precursor solution.

	Value	Unit
Process input		
chlorobenzene	9.800E-01	kg
KOH	2.765E-02	kg
H_2O	1.325E-01	kg
CH_3COOH	3.023E-02	kg
Zn	1.605E-02	kg
heat	7.244E-01	MJ
electricity	1.123E-02	kWh
Process output		
ZnO precursor solution	1.000E+00	kg
KAc	4.840E-02	kg

H_2	4.938E-04	kg
wastewater	1.370E-01	kg
waste	6.047E-04	kg

Supplementary Table 26. LCIA results for 1 kg of ZnO precursor solution.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	3.248E+00
Cumulative energy demand (MJ-Eq)	7.748E+01
Agricultural land occupation (m^2a)	1.928E-01
Climate change (kg CO_2-Eq)	2.772E+00
Fossil depletion (kg oil-Eq)	1.695E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	9.913E-02
Freshwater eutrophication (kg P-Eq)	1.386E-03
Human toxicity (kg 1,4-DCB-Eq)	5.612E+01
Ionising radiation (kg U235-Eq)	1.597E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	4.397E+01
Marine eutrophication (kg N-Eq)	2.895E-03
Metal depletion (kg Fe-Eq)	1.723E-01
Natural land transformation (m^2)	2.807E-04
Ozone depletion (kg CFC-11-Eq)	6.835E-07
Particulate matter formation (kg PM10-Eq)	8.530E-03
Photochemical oxidant formation (kg NMVOC)	2.157E-02
Terrestrial acidification (kg SO_2-Eq)	1.550E-02
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	2.961E-03
Urban land occupation (m^2a)	2.853E-02
Water depletion (m^3)	9.696E-03
Ecosystem quality (points)	1.279E-01
Human health (points)	5.002E-01
Resources (points)	2.113E-01

S3.6 FAI

$NH{=}CHNH_3I$ (FAI) is synthesized according to the technical details in a recent publication by Bi et al.[5] The LCI and the corresponding LCIA results of 1 kg of FAI are demonstrated in Supplementary Table 27 and Supplementary Table 28. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is embraced in the total heat consumption.

Supplementary Table 27. LCI for 1 kg of FAI.

	Value	Unit
Process input		
H_2O	5.763E+01	kg
iodine	3.442E+01	kg
H_2S	4.611E+00	kg
chloroform	1.828E+02	kg
Na	7.721E+01	kg
HOAc	2.039E+01	kg
NH_3	7.560E+00	kg
Ethanol	9.581E+02	kg
cooling	5.729E+00	MJ
heat	9.754E+02	MJ
electricity	1.053E+05	kWh
Process output		
$NH{=}CHNH_3I$	1.000E+00	kg
H_2	3.357E+00	kg
NaCl	1.963E+02	kg
Ethanol (chloroform)	7.460E+02	kg
wastewater	1.129E+02	kg
waste	2.114E+02	kg
Ethanol (emitted to air)	7.171E+01	kg

Supplementary Table 28. LCIA results for 1 kg of FAI.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	8.167E+01

Cumulative energy demand (MJ-Eq)	2.768E+01
Agricultural land occupation (m^2a)	1.409E+03
Climate change (kg CO_2-Eq)	6.952E-02
Fossil depletion (kg oil-Eq)	6.784E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	5.129E-02
Freshwater eutrophication (kg P-Eq)	3.462E-03
Human toxicity (kg 1,4-DCB-Eq)	2.606E+00
Ionising radiation (kg U235-Eq)	3.157E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.447E+03
Marine eutrophication (kg N-Eq)	1.369E+00
Metal depletion (kg Fe-Eq)	7.671E+01
Natural land transformation (m^2)	3.356E+01
Ozone depletion (kg CFC-11-Eq)	3.557E-01
Particulate matter formation (kg PM10-Eq)	2.704E-03
Photochemical oxidant formation (kg NMVOC)	6.397E+02
Terrestrial acidification (kg SO_2-Eq)	6.245E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	2.198E+02
Urban land occupation (m^2a)	7.560E-02
Water depletion (m^3)	4.317E-01
Ecosystem quality (points)	1.349E-02
Human health (points)	1.478E-04
Resources (points)	8.962E-02

S3.7 MABr

CH_3NH_3Br (MABr) is prepared based on the method depicted by Bi et al.[5] The LCI and the corresponding LCIA results of 1 kg of FAI are summarized in

Supplementary Table 29 and Supplementary Table 30, respectively. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is included in the total heat consumption.

Supplementary Table 29. LCI for 1 kg of MABr.

	Value	Unit
Process input		
H_2O	1.543E+03	kg
S	5.614E+01	kg
Bromine	8.421E+02	kg
CH_3NH_2	3.220E+02	kg
methanol	4.830E+02	kg
cooling	9.662E+01	MJ
heat	6.871E+03	MJ
electricity	8.725E+05	kWh
Process output		
MABr	1.000E+00	kg
H_2SO_4	1.719E+02	kg
waste	2.580E+03	kg
wastewater	4.928E+02	kg

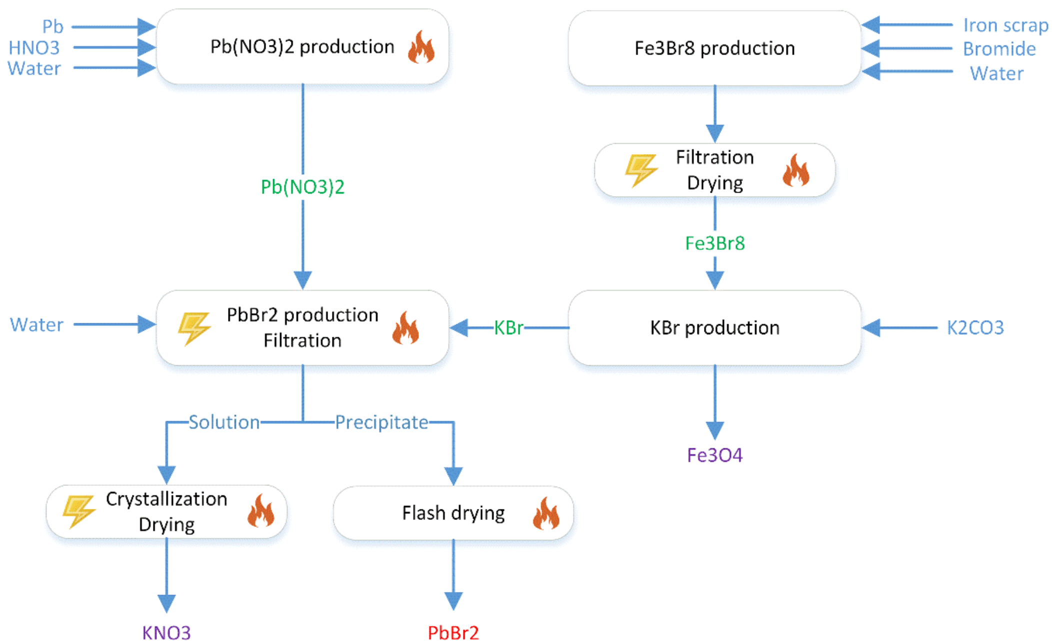
Supplementary Table 30. LCIA results for 1 kg of MABr.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	3.619E+03
Cumulative energy demand (MJ-Eq)	2.320E+02
Agricultural land occupation (m^2a)	6.318E+04
Climate change (kg CO_2-Eq)	2.312E+00
Fossil depletion (kg oil-Eq)	2.358E+02
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	2.856E-01
Freshwater eutrophication (kg P-Eq)	2.656E-02
Human toxicity (kg 1,4-DCB-Eq)	9.355E+01
Ionising radiation (kg U235-Eq)	1.036E+01
Marine ecotoxicity (kg 1,4-DCB-Eq)	6.376E+04
Marine eutrophication (kg N-Eq)	3.184E+01
Metal depletion (kg Fe-Eq)	3.416E+03

Natural land transformation (m^2)	1.505E+03
Ozone depletion (kg CFC-11-Eq)	1.497E+01
Particulate matter formation (kg PM10-Eq)	9.919E-02
Photochemical oxidant formation (kg NMVOC)	2.848E+04
Terrestrial acidification (kg SO_2-Eq)	2.324E+01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	9.592E+03
Urban land occupation (m^2a)	3.138E+00
Water depletion (m^3)	1.620E+01
Ecosystem quality (points)	5.629E-01
Human health (points)	3.044E-04
Resources (points)	3.851E+00

S3.8 $PbBr_2$

$PbBr_2$ is prepared by treating solution of lead nitrate with potassium bromide,[20] whose manufacturing route is shown in Supplementary Figure 4. A conventional method for manufacturing KBr is the reaction of potassium carbonate with Fe_3Br_8, obtained by treating scrap iron under water with excess bromine.[21] The LCI and the corresponding LCIA results of 1 kg of $PbBr_2$ are summed up in Supplementary Table 31 and Supplementary Table 32. Water consumption is reflected in the LCI, and energy consumed for distilled water generation is included in the total heat consumption.



Supplementary Figure 4. Manufacturing route for $PbBr_2$.

Supplementary Table 31. LCI for 1 kg of $PbBr_2$.

	Value	Unit
Process input		
K_2CO_3	3.760E-01	kg
iron scrap	1.144E-01	kg
bromine	4.360E-01	kg
HNO_3 (50%)	5.640E-01	kg
Pb	9.155E-01	kg
H_2O	3.777E+00	kg
heat	1.524E+01	MJ
electricity	2.399E-01	kWh
Process output		
$PbBr_2$	1.000E+00	kg
KNO_3	5.504E-01	kg
Fe_3O_4	1.580E-01	kg
CO_2	1.199E-01	kg
NO	5.450E-02	kg

wastewater	4.301E+00	kg

Supplementary Table 32. LCIA results for 1 kg of $PbBr_2$.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	3.850E+00
Cumulative energy demand (MJ-Eq)	8.288E+00
Agricultural land occupation (m^2a)	3.840E+01
Climate change (kg CO_2-Eq)	2.888E-02
Fossil depletion (kg oil-Eq)	2.540E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	4.831E-03
Freshwater eutrophication (kg P-Eq)	2.110E-03
Human toxicity (kg 1,4-DCB-Eq)	1.070E+00
Ionising radiation (kg U235-Eq)	1.466E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	5.048E+01
Marine eutrophication (kg N-Eq)	1.141E+00
Metal depletion (kg Fe-Eq)	3.537E+00
Natural land transformation (m^2)	9.154E-01
Ozone depletion (kg CFC-11-Eq)	8.717E-02
Particulate matter formation (kg PM10-Eq)	2.607E-03
Photochemical oxidant formation (kg NMVOC)	2.352E+02
Terrestrial acidification (kg SO_2-Eq)	2.037E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	1.012E+02
Urban land occupation (m^2a)	7.144E-03
Water depletion (m^3)	1.114E+00
Ecosystem quality (points)	5.770E-04
Human health (points)	3.507E-07
Resources (points)	1.946E-02

S4. LCIA results for other key components

In this section, LCIs for other key components, namely PbI_2, CH_3NH_3I, FTO glass, ITO glass, BL-TiO_2 ink, and spiro-OMeTAD are retrieved from existing publication.[1] LCI data are then converted into various impact categories by employing the LCIA method used in this work. Because the LCI for all aforementioned components are easily accessible in the literature, technical details are omitted, and only the LCIA results are summarized as follows.

S4.1 PbI_2

Supplementary Table 33. LCIA results for 1 kg of PbI_2.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	4.564E+00
Cumulative energy demand (MJ-Eq)	5.427E+01
Agricultural land occupation (m^2a)	1.047E+00
Climate change (kg CO_2-Eq)	3.898E+00
Fossil depletion (kg oil-Eq)	1.035E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	7.126E-02
Freshwater eutrophication (kg P-Eq)	1.978E-03
Human toxicity (kg 1,4-DCB-Eq)	1.559E+02
Ionising radiation (kg U235-Eq)	1.916E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	7.820E+01
Marine eutrophication (kg N-Eq)	5.158E-03
Metal depletion (kg Fe-Eq)	6.322E-01
Natural land transformation (m^2)	6.631E-04
Ozone depletion (kg CFC-11-Eq)	4.463E-07
Particulate matter formation (kg PM10-Eq)	1.105E-02
Photochemical oxidant formation (kg NMVOC)	1.555E-02
Terrestrial acidification (kg SO_2-Eq)	3.125E-02
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	5.377E-03
Urban land occupation (m^2a)	4.020E-02
Water depletion (m^3)	1.174E-02
Ecosystem quality (points)	1.912E-01
Human health (points)	1.221E+00
Resources (points)	1.534E-01

S4.2 CH_3NH_3I (MAI)

Supplementary Table 34. LCIA results for 1 kg of MAI.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	1.615E+02
Cumulative energy demand (MJ-Eq)	3.431E+03
Agricultural land occupation (m^2a)	1.614E+01
Climate change (kg CO_2-Eq)	1.478E+02
Fossil depletion (kg oil-Eq)	6.818E+01
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	5.572E+00
Freshwater eutrophication (kg P-Eq)	1.312E-01
Human toxicity (kg 1,4-DCB-Eq)	6.537E+03
Ionising radiation (kg U235-Eq)	1.580E+01
Marine ecotoxicity (kg 1,4-DCB-Eq)	4.973E+03
Marine eutrophication (kg N-Eq)	2.100E-01
Metal depletion (kg Fe-Eq)	1.181E+01
Natural land transformation (m^2)	3.118E-02
Ozone depletion (kg CFC-11-Eq)	5.345E-05
Particulate matter formation (kg PM10-Eq)	4.825E-01
Photochemical oxidant formation (kg NMVOC)	6.497E-01
Terrestrial acidification (kg SO_2-Eq)	1.224E+00
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	2.323E-01
Urban land occupation (m^2a)	2.232E+00
Water depletion (m^3)	2.899E+00
Ecosystem quality (points)	9.257E+00
Human health (points)	5.102E+01
Resources (points)	8.723E+00

S4.3 FTO glass

Supplementary Table 35. LCIA results for 1 kg of FTO glass.

Impact categories (Unit)	Value
GHG emissions (kg CO_2-Eq)	6.901E-01
Cumulative energy demand (MJ-Eq)	1.687E+01

Agricultural land occupation (m^2a)	1.230E+00
Climate change (kg CO_2-Eq)	7.116E-01
Fossil depletion (kg oil-Eq)	1.660E-01
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	1.921E-02
Freshwater eutrophication (kg P-Eq)	4.022E-04
Human toxicity (kg 1,4-DCB-Eq)	2.478E+01
Ionising radiation (kg U235-Eq)	4.365E-02
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.755E+01
Marine eutrophication (kg N-Eq)	2.106E-03
Metal depletion (kg Fe-Eq)	7.486E+00
Natural land transformation (m^2)	5.284E-04
Ozone depletion (kg CFC-11-Eq)	4.482E-08
Particulate matter formation (kg PM10-Eq)	6.202E-03
Photochemical oxidant formation (kg NMVOC)	9.550E-03
Terrestrial acidification (kg SO_2-Eq)	1.242E-02
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	1.474E-03
Urban land occupation (m^2a)	2.931E-02
Water depletion (m^3)	1.535E-03
Ecosystem quality (points)	1.012E-01
Human health (points)	2.037E-01
Resources (points)	3.674E-01

194 **S4.4 ITO glass**

195 Supplementary Table 36. LCIA results for 1 m^2 of ITO glass.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	1.684E+01
Cumulative energy demand (MJ-Eq)	2.922E+02
Agricultural land occupation (m^2a)	5.404E-02
Climate change (kg CO_2-Eq)	1.586E+01
Fossil depletion (kg oil-Eq)	6.871E+00
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	8.252E-02

Freshwater eutrophication (kg P-Eq)	1.055E-03
Human toxicity (kg 1,4-DCB-Eq)	1.655E+02
Ionising radiation (kg U235-Eq)	1.673E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	6.653E+01
Marine eutrophication (kg N-Eq)	1.505E-02
Metal depletion (kg Fe-Eq)	6.412E-01
Natural land transformation (m^2)	2.606E-03
Ozone depletion (kg CFC-11-Eq)	1.375E-06
Particulate matter formation (kg PM10-Eq)	1.995E-02
Photochemical oxidant formation (kg NMVOC)	4.886E-02
Terrestrial acidification (kg SO_2-Eq)	7.217E-02
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	7.877E-03
Urban land occupation (m^2a)	1.584E-02
Water depletion (m^3)	1.015E-02
Ecosystem quality (points)	4.891E-01
Human health (points)	1.724E+00
Resources (points)	8.537E-01

196 **S4.5 BL-TiO_2 ink**

197 Supplementary Table 37. LCIA results for 1 kg of BL-TiO_2 ink.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	1.817E+00
Cumulative energy demand (MJ-Eq)	4.924E+01
Agricultural land occupation (m^2a)	1.032E+00
Climate change (kg CO_2-Eq)	1.572E+00
Fossil depletion (kg oil-Eq)	5.645E-01
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	3.649E-02
Freshwater eutrophication (kg P-Eq)	6.776E-04
Human toxicity (kg 1,4-DCB-Eq)	2.217E+01
Ionising radiation (kg U235-Eq)	1.100E-01
Marine ecotoxicity (kg 1,4-DCB-Eq)	1.826E+01

Marine eutrophication (kg N-Eq)	6.090E-03
Metal depletion (kg Fe-Eq)	6.899E-02
Natural land transformation (m^2)	1.068E-03
Ozone depletion (kg CFC-11-Eq)	1.436E-07
Particulate matter formation (kg PM10-Eq)	4.574E-03
Photochemical oxidant formation (kg NMVOC)	5.793E-03
Terrestrial acidification (kg SO_2-Eq)	1.415E-02
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	7.737E-03
Urban land occupation (m^2a)	5.909E-02
Water depletion (m^3)	3.417E-01
Ecosystem quality (points)	3.290E-01
Human health (points)	2.157E-01
Resources (points)	7.162E-02

S4.6 Spiro-OMeTAD

Supplementary Table 38. LCIA results for 1 kg of spiro-OMeTAD.

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	1.215E+02
Cumulative energy demand (MJ-Eq)	1.958E+03
Agricultural land occupation (m^2a)	2.977E+01
Climate change (kg CO_2-Eq)	1.099E+02
Fossil depletion (kg oil-Eq)	3.547E+01
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	7.422E+00
Freshwater eutrophication (kg P-Eq)	1.279E-01
Human toxicity (kg 1,4-DCB-Eq)	6.548E+03
Ionising radiation (kg U235-Eq)	1.118E+01
Marine ecotoxicity (kg 1,4-DCB-Eq)	5.538E+03
Marine eutrophication (kg N-Eq)	1.230E-01
Metal depletion (kg Fe-Eq)	5.050E+00
Natural land transformation (m^2)	9.585E-03
Ozone depletion (kg CFC-11-Eq)	1.034E-05

Particulate matter formation (kg PM10-Eq)	6.201E-01
Photochemical oxidant formation (kg NMVOC)	4.377E-01
Terrestrial acidification (kg SO_2-Eq)	5.987E-01
Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	1.241E-01
Urban land occupation (m^2a)	1.625E+00
Water depletion (m^3)	3.610E-01
Ecosystem quality (points)	6.379E+00
Human health (points)	4.999E+01
Resources (points)	4.487E+00

S4.7 PCBM

Supplementary Table 39. LCIA results for 1 kg of PCBM.[2]

Impact categories (Unit)	**Value**
GHG emissions (kg CO_2-Eq)	6.819E+02
Cumulative energy demand (MJ-Eq)	2.096E+04
Agricultural land occupation (m^2a)	7.640E+02
Climate change (kg CO_2-Eq)	5.971E+02
Fossil depletion (kg oil-Eq)	3.481E+02
Freshwater ecotoxicity (kg 1,4-DCB-Eq)	5.378E+00
Freshwater eutrophication (kg P-Eq)	1.327E-01
Human toxicity (kg 1,4-DCB-Eq)	7.165E+03
Ionising radiation (kg U235-Eq)	2.537E+01
Marine ecotoxicity (kg 1,4-DCB-Eq)	4.742E+03
Marine eutrophication (kg N-Eq)	1.195E+00
Metal depletion (kg Fe-Eq)	1.262E+01
Natural land transformation (m^2)	8.921E-02
Ozone depletion (kg CFC-11-Eq)	4.186E-05
Particulate matter formation (kg PM10-Eq)	2.336E+00
Photochemical oxidant formation (kg NMVOC)	4.199E+00
Terrestrial acidification (kg SO_2-Eq)	3.911E+00

Terrestrial ecotoxicity (kg 1,4-DCB-Eq)	6.000E-01
Urban land occupation (m^2a)	1.271E+01
Water depletion (m^3)	1.439E+00
Ecosystem quality (points)	4.171E+01
Human health (points)	7.317E+01
Resources (points)	4.232E+01

S5. LCIA data from Ecoinvent database[3]

The characterization factors presented in this section are associated with the production process of certain material/energy, instead of the emission impacts.

Supplementary Table 40. Characterization factors for production extracted from Ecoinvent database (Part I).

item	value	unit	IPCC 2013 (kg CO_2-eq)	cumulative energy demand (MJ-eq)	ReCiPe Midpoint (E)								
					agricultural land occupation	climate change	fossil depletion	freshwater ecotoxicity	freshwater eutrophication	human toxicity	ionising radiation	marine ecotoxicity	marine eutrophication
1-Bromo-4-iodobenzene (BrC6H4I)	1	kg	3.01E+00	6.67E+01	1.18E-01	2.61E+00	1.45E+00	1.17E-01	1.31E-03	5.02E+01	1.78E-01	4.06E+01	2.65E-03
2,4,6-Trimethylaniline (C9H13N)	1	kg	5.24E+00	9.47E+01	1.31E-01	4.05E+00	2.12E+00	5.12E-02	1.47E-03	7.02E+01	1.88E-01	5.25E+01	5.66E-03
2-Methoxyethanol (C3H8O2)	1	kg	2.34E+00	6.58E+01	8.03E-02	2.08E+00	1.46E+00	1.82E-02	7.81E-04	2.75E+01	1.22E-01	2.16E+01	1.69E-03
4-tert-Butylpyridine (C9H13N)	1	kg	1.11E+01	1.82E+02	6.17E-01	1.02E+01	3.73E+00	1.45E-01	4.76E-03	2.15E+02	9.00E-01	1.70E+02	1.25E-02
Acetic acid (CH3COOH, 98%)	1	kg	1.87E+00	5.09E+01	7.77E-02	1.57E+00	1.13E+00	2.49E-02	7.47E-04	3.94E+01	2.01E-01	2.64E+01	1.57E-03
Acetic anhydride (C4H6O3)	1	kg	3.97E+00	7.90E+01	1.94E-01	3.54E+00	1.72E+00	4.33E-02	1.30E-03	6.58E+01	3.41E-01	4.62E+01	2.93E-03
Acetone (C3H6O)	1	kg	2.32E+00	6.74E+01	3.82E-04	1.93E+00	1.54E+00	1.63E-02	1.56E-04	1.06E+00	3.09E-04	2.09E+00	1.81E-03
Acetonitrile (C2H3N)	1	kg	4.08E+00	1.10E+02	6.15E-02	3.68E+00	2.54E+00	1.75E-02	4.29E-04	2.87E+01	8.83E-02	2.24E+01	1.68E-02
Alumina (Al2O3)	1	kg	1.26E+00	1.54E+01	2.04E-02	1.19E+00	3.45E-01	4.02E-02	5.43E-04	4.22E+01	5.83E-02	6.23E+01	1.31E-03
Aluminium (Al)	1	kg	2.66E+01	2.48E+02	3.70E-01	2.45E+01	5.51E+00	2.38E-01	6.70E-03	2.99E+02	2.63E-01	3.19E+02	2.36E-02
Aniline (C6H5NH2)	1	kg	5.24E+00	9.47E+01	1.31E-01	4.05E+00	2.12E+00	5.12E-02	1.47E-03	7.02E+01	1.88E-01	5.25E+01	5.66E-03
Argon (Ar)	1	kg	2.69E+00	4.04E+01	1.41E-01	2.49E+00	7.14E-01	3.53E-02	1.46E-03	4.68E+01	4.14E-01	4.03E+01	2.43E-03
Barite (BaSO4)	1	kg	2.90E-01	3.97E+00	1.49E-02	2.68E-01	7.60E-02	3.87E-03	1.50E-04	5.61E+00	2.91E-02	4.51E+00	2.86E-04
Benzaldehyde (C7H6O)	1	kg	5.16E+00	1.10E+02	2.81E-01	4.64E+00	2.33E+00	5.02E-02	1.75E-03	7.68E+01	4.06E-01	5.89E+01	4.15E-03
Benzene (C6H6)	1	kg	1.86E+00	6.76E+01	2.07E-04	1.56E+00	1.56E+00	1.27E-03	1.40E-05	7.03E-01	1.76E-04	2.07E+00	1.10E-03
Bis(trimethylsilyl)amine ([(CH3)3Si]2NH)	1	kg	5.74E+00	1.01E+02	4.98E-01	5.22E+00	2.03E+00	6.16E-02	1.83E-03	8.34E+01	4.31E-01	9.04E+01	1.16E-02
Bromine (Br2)	1	kg	5.02E+00	6.62E+01	1.02E-01	4.72E+00	1.47E+00	3.36E-02	1.20E-03	5.53E+01	2.57E-01	4.15E+01	3.34E-03
Calcium chloride (CaCl2)	1	kg	9.14E-01	1.03E+01	1.19E-01	8.40E-01	2.04E-01	1.51E-02	4.44E-04	1.99E+01	4.76E-02	1.50E+01	1.23E-03
Chlorine (Cl2)	1	kg	2.21E-01	3.02E+00	1.19E-02	2.05E-01	5.96E-02	2.98E-03	1.06E-04	4.56E+00	2.07E-02	3.49E+00	2.34E-04
Chlorobenzene (C6H5Cl)	1	kg	3.24E+00	7.85E+01	1.15E-01	2.76E+00	1.73E+00	1.01E-01	1.33E-03	5.04E+01	1.55E-01	4.10E+01	2.73E-03
Citric acid (C6H8O7)	1	kg	2.85E+00	6.89E+01	1.20E+00	2.56E+00	7.62E-01	5.04E-02	1.37E-03	4.66E+01	4.67E-01	3.76E+01	8.92E-03
Coal	1	kg	2.20E+00	5.75E+01	6.82E+00	7.17E-01	1.76E-01	4.81E-03	9.96E-05	4.25E+00	3.85E-02	4.08E+00	9.02E-04
Coal tar	1	kg	5.11E+02	7.79E+03	2.37E+01	4.59E+02	1.48E+02	1.39E+01	2.87E-01	9.48E+03	6.15E+01	9.83E+03	4.62E-01
Cooling	1	MJ	1.55E-01	2.48E+00	1.82E-03	1.41E-01	5.59E-02	1.24E-03	2.65E-05	1.39E+00	5.35E-03	1.06E+00	5.06E-05
Cullet	1	kg	1.40E-02	1.46E-01	5.89E-04	1.07E-02	2.83E-03	5.99E-04	2.67E-06	2.31E-01	1.27E-03	1.29E+00	3.30E-05
Deionised water	1	kg	1.74E-03	2.40E-02	8.02E-05	1.60E-03	4.61E-04	2.40E-05	8.52E-07	3.19E-02	1.74E-04	2.74E-02	1.72E-06
Diethyl ether ((C2H5)2O)	1	kg	7.01E+00	1.55E+02	4.14E-01	6.39E+00	3.22E+00	1.08E-01	4.09E-03	1.75E+02	7.85E-01	1.27E+02	8.08E-03
Dimethyl sulfate (C2H6O4S)	1	kg	1.36E+00	3.78E+01	8.42E-02	1.22E+00	8.24E-01	2.91E-02	7.86E-04	5.08E+01	1.40E-01	3.16E+01	1.59E-03
Dimethylformamide (C3H7NO, DMF)	1	kg	2.86E+00	7.78E+01	1.16E-01	2.59E+00	1.74E+00	3.64E-02	9.83E-04	5.94E+01	2.56E-01	3.86E+01	1.25E-02
Dioxane (C4H8O2)	1	kg	5.04E+00	1.06E+02	2.29E-01	4.57E+00	2.30E+00	4.35E-02	1.53E-03	6.74E+01	2.97E-01	5.25E+01	3.84E-03
Dolomite	1	kg	4.21E-02	5.16E-01	2.27E-03	3.87E-02	1.03E-02	4.28E-04	1.75E-05	6.16E-01	3.04E-03	5.26E-01	5.39E-05
Electricity	1	kWh	7.10E-01	1.25E+01	8.13E-04	6.70E-01	2.96E-01	2.55E-03	1.24E-05	5.22E+00	4.22E-03	1.57E+00	6.15E-04
Ethanol (C2H6O)	1	kg	1.40E+00	4.16E+01	1.12E+00	1.22E+00	3.43E-01	3.41E-02	5.68E-04	1.67E+01	8.71E-02	1.34E+01	6.24E-03
Ethyl acetate (C4H8O2)	1	kg	2.86E+00	7.37E+01	1.50E-01	2.50E+00	1.64E+00	2.79E-02	1.07E-03	4.50E+01	1.94E-01	3.18E+01	2.30E-03
Ethylene glycol (C2H6O2)	1	kg	1.99E+00	5.39E+01	7.47E-02	1.77E+00	1.17E+00	1.88E-02	6.43E-04	2.79E+01	1.44E-01	2.22E+01	1.53E-03
Ethylenediamine (C2H8N2)	1	kg	6.14E+00	1.19E+02	3.05E-01	5.66E+00	2.44E+00	8.14E-02	2.55E-03	1.17E+02	6.40E-01	9.11E+01	1.74E-02
Ethylenediaminetetraacetic acid (C10H16N2O8, EDTA)	1	kg	4.21E+00	8.17E+01	1.58E-01	3.67E+00	1.74E+00	6.99E-02	1.39E-03	6.65E+01	3.02E-01	4.93E+01	1.38E-02
Ferrous chloride (FeCl2)	1	kg	2.39E-01	3.52E+00	2.60E-02	2.21E-01	6.19E-02	6.28E-03	1.95E-04	1.03E+01	3.24E-02	7.34E+00	2.46E-04
Gold (Au)	1	kg	1.75E+04	2.72E+05	4.00E+02	1.66E+04	5.53E+03	3.19E+04	9.64E+02	7.64E+07	2.59E+03	3.81E+07	1.20E+02
Heat	1	MJ	2.26E-02	1.13E+00	1.12E-01	1.86E-02	6.38E-03	4.35E-04	1.04E-05	5.32E-01	1.83E-03	3.53E-01	1.23E-04
Hexanes (C6H14)	1	kg	6.10E-01	2.40E+01	3.95E-02	5.72E-01	5.49E-01	8.33E-03	2.19E-04	1.46E+01	1.10E-01	9.52E+00	5.52E-04
Hydrochloric acid (HCl, 30%)	1	kg	1.72E+00	2.49E+01	1.01E-01	1.58E+00	4.79E-01	2.67E-02	9.55E-04	4.05E+01	1.75E-01	3.11E+01	1.73E-03
Hydrogen (H2)	1	kg	2.04E+01	2.80E+02	1.10E+00	1.88E+01	5.32E+00	2.95E-01	1.10E-02	4.28E+02	2.14E+00	3.41E+02	2.08E-02
Hydrogen fluoride (HF)	1	kg	3.50E+00	7.43E+01	2.67E-01	3.24E+00	1.51E+00	8.13E-02	2.59E-03	1.43E+02	4.99E-01	9.71E+01	5.45E-03
Hydrogen peroxide (H2O2, 50%)	1	kg	1.25E+00	2.01E+01	5.41E-02	1.11E+00	4.27E-01	3.01E-02	4.49E-04	2.17E+01	7.61E-02	5.02E+01	1.15E-03

Hydrogen sulfide (H2S)	**1**	**kg**	4.69E-01	9.75E+00	2.92E-02	4.14E-01	2.05E-01	7.61E-03	2.44E-04	1.22E+01	3.61E-02	8.90E+00	4.08E-04
Incineration of average residue	**1**	**kg**	3.69E-01	2.37E+00	6.09E-03	3.59E-01	5.20E-02	1.22E-01	1.86E-03	1.14E+02	1.05E-02	9.15E+01	2.90E-04
Indium (In)	**1**	**kg**	2.19E+02	2.55E+03	7.48E+00	2.00E+02	5.18E+01	8.59E+00	2.56E-01	1.82E+04	8.06E+00	1.05E+04	3.69E-01
Iodine (I2)	**1**	**kg**	5.01E+00	6.58E+01	1.01E-01	4.71E+00	1.46E+00	3.32E-02	1.18E-03	5.45E+01	2.55E-01	4.09E+01	3.32E-03
Isopropyl alcohol (C3H8O)	**1**	**kg**	1.83E+00	6.04E+01	3.67E-02	1.59E+00	1.38E+00	9.28E-03	2.63E-04	1.53E+01	3.69E-02	1.14E+01	1.12E-03
Lanthanum oxide (La2O3)	**1**	**kg**	1.86E+01	3.89E+02	1.13E+00	1.72E+01	8.46E+00	4.60E-01	8.02E-03	4.51E+02	1.59E+00	2.99E+02	1.52E-02
Lead (Pb)	**1**	**kg**	1.67E+00	1.67E+01	1.18E-01	1.55E+00	3.46E-01	1.17E-01	3.40E-03	3.70E+02	7.03E-02	1.38E+02	4.01E-03
Li (Lithium)	**1**	**kg**	5.99E+01	8.19E+02	3.86E+00	5.57E+01	1.53E+01	8.46E-01	3.67E-02	1.20E+03	6.79E+00	9.41E+02	9.32E-02
Limestone	**1**	**kg**	3.10E-03	4.32E-02	6.60E-05	2.82E-03	9.42E-04	1.60E-05	4.67E-07	2.26E-02	2.02E-04	1.84E-02	2.03E-05
Liquid Ammonia (NH3)	**1**	**kg**	1.87E+00	3.78E+01	2.29E-02	1.78E+00	8.84E-01	1.24E-02	1.76E-04	2.23E+01	6.68E-02	1.43E+01	9.04E-04
Lithium carbonate (Li2CO3)	**1**	**kg**	2.54E+00	3.53E+01	2.52E-01	2.37E+00	7.11E-01	4.08E-02	2.27E-03	5.76E+01	2.07E-01	4.16E+01	9.00E-03
Magnesium (Mg)	**1**	**kg**	1.68E+01	2.77E+02	7.55E-02	1.51E+01	6.47E+00	3.48E-02	8.59E-04	5.24E+01	2.67E-01	3.24E+01	4.85E-03
Mercury (Hg)	**1**	**kg**	1.66E+01	1.51E+02	1.60E+00	1.52E+01	3.27E+00	1.93E+00	4.50E-03	1.97E+05	2.10E-01	1.17E+04	1.38E-02
Methane (CH4)	**1**	**kg**	3.50E+00	2.89E+01	2.62E-01	2.13E+00	5.15E-01	1.56E-01	4.39E-03	5.27E+01	2.28E-01	7.19E+01	3.78E-03
Methanol (CH3OH)	**1**	**kg**	6.93E-01	6.96E+01	8.08E+00	6.39E-01	2.08E-01	1.37E-02	4.67E-04	2.28E+01	7.82E-02	1.34E+01	1.13E-03
Methylamine (CH5N)	**1**	**kg**	2.56E+00	6.86E+01	6.12E-02	2.33E+00	1.58E+00	2.78E-02	5.58E-04	4.79E+01	1.25E-01	2.83E+01	3.94E-03
n-Butanol (C4H10O)	**1**	**kg**	3.14E+00	8.37E+01	1.27E-01	2.76E+00	1.88E+00	2.28E-02	8.21E-04	3.56E+01	1.80E-01	2.80E+01	2.37E-03
Nickel (II) sulfate (NiSO4)	**1**	**kg**	5.18E+00	7.38E+01	3.23E-01	4.82E+00	1.36E+00	8.87E-01	1.30E-02	9.65E+02	4.30E-01	1.04E+03	1.20E-02
Nitric acid (HNO3, 50%)	**1**	**kg**	2.91E+00	1.30E+01	2.51E-02	1.94E+00	2.97E-01	7.93E-03	1.65E-04	1.41E+01	3.65E-02	9.83E+00	2.62E-03
Nitrogen (N2)	**1**	**kg**	4.70E-01	6.40E+00	1.85E-02	4.34E-01	1.23E-01	5.67E-03	2.30E-04	7.67E+00	4.77E-02	6.56E+00	4.29E-04
Oxygen (O2)	**1**	**kg**	1.18E+00	1.61E+01	4.66E-02	1.09E+00	3.09E-01	1.43E-02	5.81E-04	1.93E+01	1.20E-01	1.65E+01	1.08E-03
Palladium (Pd)	**1**	**kg**	4.05E+03	6.56E+04	1.28E+02	3.75E+03	1.27E+03	4.49E+02	3.06E+00	1.82E+05	6.64E+02	4.97E+05	3.61E+00
Phenol (C6H5OH)	**1**	**kg**	4.60E+00	1.20E+02	1.11E-01	3.95E+00	2.69E+00	3.75E-02	1.37E-03	5.22E+01	1.68E-01	4.31E+01	3.24E-03
Phosphorus trichloride (PCl3)	**1**	**kg**	4.53E+00	6.96E+01	2.77E-01	3.91E+00	1.29E+00	7.51E-02	2.62E-03	8.89E+01	6.85E-01	7.29E+01	4.70E-03
Potassium hydroxide (KOH)	**1**	**kg**	2.36E+00	3.21E+01	1.30E-01	2.18E+00	6.42E-01	2.97E-02	1.09E-03	4.49E+01	1.84E-01	3.52E+01	2.13E-03
Potassium iodate (KIO3)	**1**	**kg**	4.94E+00	6.67E+01	2.19E-01	4.52E+00	1.27E+00	8.41E-02	2.50E-03	9.09E+01	5.01E-01	1.16E+02	4.84E-03
Potassium iodide (KI)	**1**	**kg**	5.32E-01	9.49E+00	3.94E-02	4.86E-01	1.94E-01	8.79E-03	2.28E-04	1.47E+01	3.17E-02	9.99E+00	4.67E-04
Silica sand	**1**	**kg**	3.92E-02	4.34E-01	2.80E-03	3.63E-02	9.46E-03	2.39E-04	1.01E-05	4.00E-01	1.45E-03	3.43E-01	5.04E-05
Sodium (Na)	**1**	**kg**	2.02E+00	2.76E+01	1.09E-01	1.88E+00	5.45E-01	2.72E-02	9.65E-04	4.17E+01	1.89E-01	3.19E+01	2.14E-03
Sodium carbonate (Na2CO3)	**1**	**kg**	6.00E-01	6.79E+00	7.83E-02	5.51E-01	1.34E-01	9.89E-03	2.91E-04	1.31E+01	3.12E-02	9.84E+00	8.06E-04
Sodium chloride (NaCl)	**1**	**kg**	2.63E-01	3.39E+00	2.68E-02	2.43E-01	6.36E-02	6.14E-03	1.95E-04	1.02E+01	2.33E-02	7.23E+00	3.63E-04
Sodium hydroxide (NaOH, 50%)	**1**	**kg**	1.45E+00	2.00E+01	7.82E-02	1.34E+00	3.79E-01	2.10E-02	7.82E-04	3.05E+01	1.52E-01	2.43E+01	1.48E-03
Sodium methoxide (CH3ONa)	**1**	**kg**	1.86E+00	4.22E+01	1.01E-01	1.68E+00	8.81E-01	3.00E-02	9.24E-04	4.69E+01	2.08E-01	3.18E+01	1.80E-03
Sodium nitrite (NaNO2)	**1**	**kg**	3.05E+00	4.78E+01	1.56E-01	2.85E+00	9.37E-01	3.92E-02	1.36E-03	5.90E+01	3.62E-01	4.62E+01	5.20E-03
Sulfur dioxide (SO2)	**1**	**kg**	4.94E-01	2.06E+01	3.02E-02	4.54E-01	4.64E-01	8.42E-03	2.58E-04	1.37E+01	9.51E-02	9.61E+00	5.55E-04
Sulfuric acid (H2SO4)	**1**	**kg**	1.14E-01	6.97E+00	1.26E-02	1.04E-01	1.59E-01	3.39E-03	8.21E-05	5.73E+00	2.96E-02	4.08E+00	3.46E-04
Sulfuryl chloride (SO2Cl2)	**1**	**kg**	1.62E+00	3.85E+01	1.13E-01	1.50E+00	7.85E-01	2.82E-02	9.49E-04	4.37E+01	2.67E-01	3.22E+01	1.69E-03
tert-Butyl alcohol (C4H10O)	**1**	**kg**	3.40E+00	8.11E+01	2.15E-01	3.07E+00	1.85E+00	2.24E-02	8.06E-04	4.02E+01	6.85E-02	2.91E+01	2.62E-03
Tetrahydrofuran (C4H8O)	**1**	**kg**	6.71E+00	1.17E+02	4.64E-01	6.12E+00	2.45E+00	7.60E-02	2.57E-03	1.19E+02	4.72E-01	8.67E+01	5.83E-03
Tetramethylethylenediamine (C6H16N2, TMEDA)	**1**	**kg**	6.14E+00	1.19E+02	3.05E-01	5.66E+00	2.44E+00	8.14E-02	2.55E-03	1.17E+02	6.40E-01	9.11E+01	1.74E-02
Tin (Sn)	**1**	**kg**	2.41E+01	3.19E+02	8.40E-01	2.23E+01	6.41E+00	2.44E-01	9.44E-03	3.42E+02	2.07E+00	2.82E+02	6.04E-02
Titanium dioxide (TiO2)	**1**	**kg**	8.60E+00	9.22E+01	3.68E-01	7.43E+00	1.83E+00	1.32E-01	3.41E-03	1.21E+02	4.63E-01	1.52E+02	7.91E-03
Titanium tetrachloride (TiCl4)	**1**	**kg**	3.34E+00	3.60E+01	1.39E-01	2.67E+00	7.19E-01	4.61E-02	1.55E-03	5.43E+01	2.29E-01	6.06E+01	3.12E-03
Toluene (C7H8)	**1**	**kg**	1.56E+00	6.34E+01	1.57E-04	1.28E+00	1.47E+00	8.85E-04	1.03E-05	5.14E-01	1.32E-04	1.32E+00	8.13E-04
Treatment of wastewater	**1**	**t**	2.48E+00	2.07E+01	8.89E-02	2.26E+00	3.91E-01	3.46E-02	1.41E-02	3.20E+01	1.59E-01	3.11E+01	1.30E-01
Trimethyl borate (C3H9BO3)	**1**	**kg**	1.64E+00	5.06E+01	5.96E-02	1.45E+00	1.16E+00	2.65E-02	5.90E-04	4.76E+01	9.60E-02	2.62E+01	2.15E-03
Urea (CH4N2O)	**1**	**kg**	3.32E+00	6.06E+01	7.99E-02	3.13E+00	1.39E+00	2.89E-02	6.03E-04	5.00E+01	1.63E-01	3.55E+01	2.52E-03
Xylene (C8H10)	**1**	**kg**	1.70E+00	6.58E+01	1.81E-04	1.41E+00	1.52E+00	1.38E-03	1.37E-05	6.98E-01	1.59E-04	2.65E+00	9.28E-04
Zinc (Zn)	**1**	**kg**	5.09E+00	5.86E+01	1.71E-01	4.63E+00	1.19E+00	1.92E-01	5.69E-03	4.06E+02	1.72E-01	2.36E+02	8.68E-03

Supplementary Table 41. Characterization factors for production extracted from Ecoinvent database (Part II).

item	**ReCiPe Midpoint (E)**									**ReCiPe Endpoint (E,A)**		
	metal depletion	**natural land transformation**	**ozone depletion**	**particulate matter formation**	**photochemical oxidant formation**	**terrestrial acidification**	**terrestrial ecotoxicity**	**urban land occupation**	**water depletion**	**ecosystem quality**	**human health**	**resources**
1-Bromo-4-iodobenzene (BrC6H4I)	1.29E-01	2.65E-04	8.50E-07	8.13E-03	1.80E-02	1.41E-02	2.07E-03	2.55E-02	8.44E-03	1.18E-01	4.53E-01	1.79E-01
2,4,6-Trimethylaniline (C9H13N)	2.55E-01	5.47E-04	3.05E-07	1.09E-02	1.96E-02	3.00E-02	3.43E-03	3.60E-02	7.55E-03	1.70E-01	6.49E-01	2.66E-01
2-Methoxyethanol (C3H8O2)	1.03E-01	1.68E-04	7.69E-08	3.91E-03	8.06E-03	8.48E-03	9.78E-04	1.22E-02	4.41E-03	7.97E-02	2.69E-01	1.80E-01
4-tert-Butylpyridine (C9H13N)	6.75E-01	1.49E-03	2.81E-06	2.87E-02	3.17E-02	5.62E-02	1.04E-02	9.08E-02	3.26E-02	4.59E-01	1.89E+00	4.79E-01
Acetic acid (CH3COOH, 98%)	1.03E-01	7.77E-04	3.63E-07	5.14E-03	7.19E-03	1.08E-02	1.31E-03	1.43E-02	5.93E-03	7.40E-02	3.35E-01	1.40E-01
Acetic anhydride (C4H6O3)	1.82E-01	1.18E-03	5.41E-07	8.34E-03	1.23E-02	1.96E-02	2.55E-03	2.86E-02	1.11E-02	1.53E-01	5.89E-01	2.15E-01
Acetone (C3H6O)	1.24E-03	-1.88E-07	9.56E-10	2.80E-03	9.06E-03	1.02E-02	1.79E-04	1.65E-04	1.38E-04	5.34E-02	8.31E-02	1.85E-01

Acetonitrile (C2H3N)	1.08E-01	4.15E-04	1.99E-07	6.24E-03	9.43E-03	2.64E-02	2.46E-03	9.83E-03	9.46E-03	1.23E-01	3.39E-01	3.09E-01
Alumina (Al2O3)	6.99E-02	1.51E-04	1.49E-07	3.09E-03	4.18E-03	4.18E-03	1.16E-03	1.16E-03	1.91E-03	5.97E-02	3.35E-01	4.46E-02
Aluminium (Al)	2.66E-01	1.65E-03	7.15E-07	5.55E-02	7.19E-02	1.32E-01	6.21E-03	1.95E-01	6.61E-02	1.02E+00	3.02E+00	6.73E-01
Aniline (C6H5NH2)	2.55E-01	5.47E-04	3.05E-07	1.09E-02	1.96E-02	3.00E-02	3.43E-03	3.60E-02	7.55E-03	1.70E-01	6.49E-01	2.66E-01
Argon (Ar)	3.24E-02	2.95E-04	1.49E-07	8.33E-03	6.63E-03	1.31E-02	8.99E-04	1.60E-02	1.05E-02	1.06E-01	4.25E-01	8.71E-02
Barite (BaSO4)	8.77E-03	3.69E-05	1.49E-08	9.88E-04	7.96E-04	1.50E-03	1.31E-04	2.32E-03	1.19E-03	1.24E-02	5.00E-02	9.52E-03
Benzaldehyde (C7H6O)	2.46E-01	4.98E-04	1.18E-06	1.00E-02	1.58E-02	2.21E-02	4.78E-03	3.66E-02	1.09E-02	1.93E-01	7.06E-01	2.90E-01
Benzene (C6H6)	1.03E-03	-2.15E-07	5.38E-10	1.79E-03	5.67E-03	6.23E-03	5.02E-04	1.04E-04	1.56E-04	4.32E-02	6.43E-02	1.87E-01
Bis(trimethylsilyl)amine ([(CH3)3Si]2NH)	3.77E-01	8.64E-04	3.94E-06	1.30E-02	1.72E-02	2.97E-02	4.11E-03	5.03E-02	1.70E-02	2.27E-01	7.81E-01	2.61E-01
Bromine (Br2)	1.17E-01	1.03E-03	8.04E-07	8.44E-03	1.07E-02	2.25E-02	7.13E-03	2.54E-02	8.82E-03	1.79E-01	5.55E-01	1.82E-01
Calcium chloride (CaCl2)	7.90E-02	9.69E-05	4.39E-08	2.63E-03	2.78E-03	9.26E-03	8.81E-04	1.14E-02	1.85E-03	4.25E-02	1.69E-01	2.81E-02
Chlorine (Cl2)	1.46E-02	3.58E-05	1.57E-08	6.12E-04	6.10E-04	1.15E-03	2.34E-04	2.27E-03	6.57E-04	9.67E-03	3.96E-02	7.83E-03
Chlorobenzene (C6H5Cl)	1.33E-01	2.54E-04	7.11E-07	8.27E-03	2.19E-02	1.48E-02	1.90E-03	2.70E-02	8.47E-03	1.23E-01	4.60E-01	2.14E-01
Citric acid (C6H8O7)	1.59E-01	1.07E-03	3.30E-07	6.25E-03	7.71E-03	2.35E-02	7.26E-03	5.98E-02	3.76E-01	3.56E-01	4.20E-01	9.88E-02
Coal	2.10E-02	1.80E-04	7.37E-08	1.66E-03	1.81E-02	2.84E-03	7.21E-04	9.00E-02	8.79E-04	1.91E-01	5.71E-02	2.21E-02
Coal tar	2.47E+01	5.57E-02	3.09E-05	3.45E+00	1.71E+00	2.49E+00	3.01E-01	4.41E+00	1.90E+00	2.17E+01	8.91E+01	1.89E+01
Cooling	5.85E-03	2.37E-05	1.75E-08	1.52E-04	2.24E-04	3.47E-04	4.56E-05	3.15E-04	1.69E-03	4.63E-03	1.47E-02	6.98E-03
Cullet	8.26E-04	-3.44E-07	1.52E-09	2.42E-05	4.41E-05	4.87E-05	2.98E-05	5.49E-04	4.11E-05	9.36E-04	1.99E-03	3.78E-04
Deionised water	1.15E-04	2.21E-07	7.30E-10	5.70E-06	4.90E-06	8.82E-06	1.43E-06	1.53E-05	1.31E-03	7.51E-05	2.87E-04	6.06E-05
Diethyl ether ((C2H5)2O)	5.96E-01	1.30E-03	2.74E-06	2.29E-02	3.04E-02	5.68E-02	7.27E-03	7.83E-02	2.31E-02	3.06E-01	1.48E+00	4.13E-01
Dimethyl sulfate (C2H6O4S)	1.93E-01	4.89E-04	2.27E-07	5.20E-03	6.01E-03	1.54E-02	1.71E-03	1.89E-02	5.16E-03	6.65E-02	4.04E-01	1.08E-01
Dimethylformamide (C3H7NO, DMF)	1.67E-01	1.09E-03	5.20E-07	7.22E-03	8.76E-03	1.84E-02	1.84E-02	2.21E-02	7.74E-03	1.15E-01	5.12E-01	2.17E-01
Dioxane (C4H8O2)	2.03E-01	4.76E-04	1.94E-07	9.72E-03	1.41E-02	2.15E-02	2.36E-03	3.14E-02	1.00E-02	1.84E-01	6.39E-01	2.85E-01
Dolomite	1.35E-03	4.66E-06	1.83E-09	1.90E-04	1.59E-04	2.65E-04	1.67E-05	3.51E-04	1.45E-04	1.63E-03	5.97E-03	1.30E-03
Electricity	3.00E-03	1.10E-04	5.93E-08	7.49E-04	2.01E-03	2.90E-03	5.19E-05	3.20E-04	8.02E-05	1.96E-02	6.05E-02	3.56E-02
Ethanol (C2H6O)	5.45E-02	1.05E-03	8.90E-08	3.92E-03	4.11E-03	1.29E-02	8.21E-03	5.98E-02	3.74E-01	3.41E-01	1.65E-01	4.36E-02
Ethyl acetate (C4H8O2)	1.45E-01	7.19E-04	3.25E-07	5.73E-03	1.19E-02	1.47E-02	1.84E-03	2.12E-02	6.99E-03	1.07E-01	4.05E-01	2.04E-01
Ethylene glycol (C2H6O2)	9.64E-02	1.39E-04	6.81E-08	3.89E-03	6.08E-03	7.62E-03	8.88E-04	1.11E-02	4.06E-03	7.10E-02	2.61E-01	1.45E-01
Ethylenediamine (C2H8N2)	3.77E-01	9.63E-04	2.23E-06	1.53E-02	1.69E-02	3.31E-02	3.92E-02	5.19E-02	1.59E-02	2.58E-01	1.03E+00	3.10E-01
Ethylenediaminetetraacetic acid (C10H16N2O8, EDTA)	2.23E-01	5.78E-04	8.81E-07	8.65E-03	1.14E-02	2.04E-02	9.15E-03	2.94E-02	1.01E-02	1.54E-01	6.02E-01	2.19E-01
Ferrous chloride (FeCl2)	5.01E-02	3.83E-05	1.85E-08	8.08E-04	6.83E-04	1.41E-03	3.20E-04	3.32E-03	9.59E-04	1.39E-02	7.99E-02	9.75E-03
Gold (Au)	7.99E+04	1.13E+01	2.45E-03	8.88E+01	2.20E+02	2.04E+02	3.01E+01	2.56E+03	2.17E+02	1.17E+04	5.23E+05	4.37E+03
Heat	1.18E-03	6.10E-06	1.77E-09	2.40E-04	4.16E-04	3.10E-04	7.43E-05	1.75E-03	5.75E-05	3.97E-03	4.55E-03	8.19E-04
Hexanes (C6H14)	7.44E-02	5.55E-04	2.67E-07	1.33E-03	6.61E-03	3.60E-03	6.29E-04	6.29E-04	1.30E-03	3.00E-02	1.22E-01	6.93E-02
Hydrochloric acid (HCl, 30%)	1.19E-01	2.18E-04	7.36E-07	5.62E-03	4.71E-03	9.00E-03	2.18E-03	1.60E-02	6.08E-03	7.61E-02	3.45E-01	6.30E-02
Hydrogen (H2)	9.98E-01	2.59E-03	1.05E-05	6.76E-02	5.54E-02	1.07E-01	1.23E-02	1.78E-01	7.34E-02	8.83E-01	3.74E+00	6.84E-01
Hydrogen fluoride (HF)	5.39E-01	1.14E-03	5.32E-07	1.78E-02	1.81E-02	5.23E-02	4.78E-03	5.01E-02	1.41E-02	1.81E-01	1.14E+00	2.07E-01
Hydrogen peroxide (H2O2, 50%)	7.88E-02	1.79E-04	9.89E-08	2.81E-03	3.48E-03	5.44E-03	6.23E-04	7.73E-03	5.28E-03	5.51E-02	1.93E-01	5.48E-02
Hydrogen sulfide (H2S)	5.29E-02	5.14E-05	4.50E-08	1.29E-03	1.29E-03	2.21E-03	3.72E-04	4.12E-03	1.35E-03	2.08E-02	1.01E-01	2.70E-02
Incineration of average residue	5.65E-03	-8.05E-05	1.85E-08	4.20E-04	8.72E-04	9.91E-04	1.28E-03	1.26E-02	4.77E-04	3.45E-02	7.91E-01	6.50E-03
Indium (In)	1.18E+02	3.00E-02	8.76E-06	8.53E-01	1.14E+00	2.22E+00	2.85E+00	2.41E+00	3.02E+00	1.37E+01	1.33E+02	1.17E+01
Iodine (I2)	1.13E-01	1.02E-03	8.01E-07	8.35E-03	1.06E-02	2.21E-02	7.09E-03	2.51E-02	8.77E-03	1.79E-01	5.49E-01	1.81E-01
Isopropyl alcohol (C3H8O)	6.46E-02	1.47E-04	6.47E-08	2.41E-03	7.86E-03	6.76E-03	5.24E-04	5.21E-03	4.23E-03	5.49E-02	1.66E-01	1.69E-01
Lanthanum oxide (La2O3)	1.59E+00	6.31E-03	4.23E-06	5.58E-02	5.20E-02	8.89E-02	6.42E-02	1.60E-01	6.94E-02	8.09E-01	3.81E+00	1.09E+00
Lead (Pb)	1.89E+00	2.20E-04	8.35E-08	1.03E-02	1.26E-02	3.83E-02	3.00E-03	2.33E-02	1.88E-02	1.17E-01	2.60E+00	1.29E-01
Li (Lithium)	2.84E+00	9.15E-03	7.41E-06	1.76E-01	1.72E-01	3.33E-01	4.65E-02	1.18E+00	1.92E-01	3.58E+00	1.05E+01	1.97E+00
Limestone	1.66E-04	9.32E-07	4.14E-10	7.47E-05	6.08E-05	5.58E-05	1.55E-06	9.91E-05	1.92E-04	1.06E-04	4.40E-04	1.21E-04
Liquid Ammonia (NH3)	7.00E-02	5.07E-04	2.54E-07	2.40E-03	3.36E-03	7.43E-03	2.57E-03	4.48E-03	9.70E-04	6.14E-02	2.19E-01	1.09E-01
Lithium carbonate (Li2CO3)	1.96E-01	7.00E-04	2.54E-07	7.42E-03	1.10E-02	2.05E-02	3.38E-03	1.44E-01	5.91E-03	2.89E-01	4.90E-01	9.44E-02
Magnesium (Mg)	1.39E-01	2.85E-03	2.10E-06	9.15E-03	2.36E-02	2.94E-02	1.26E-03	2.97E-02	4.68E-02	4.90E-01	8.99E-01	7.82E-01
Mercury (Hg)	6.91E-02	1.05E-03	3.32E-07	3.33E-02	4.39E-02	1.05E-01	2.73E+02	1.15E-01	1.72E-02	6.35E+01	1.35E+03	3.95E-01
Methane (CH4)	1.18E-01	5.49E-04	1.41E-07	6.33E-03	8.23E-03	1.39E-02	2.71E-03	2.70E-02	1.58E-02	1.11E-01	4.48E-01	6.73E-02
Methanol (CH3OH)	4.43E-02	1.83E-04	7.24E-08	2.38E-03	3.64E-03	4.22E-03	1.09E-03	5.58E-02	4.68E-03	2.28E-01	1.71E-01	2.70E-02
Methylamine (CH5N)	1.31E-01	8.45E-04	4.05E-07	5.53E-03	7.18E-03	1.83E-02	3.03E-03	1.48E-02	4.99E-03	9.38E-02	4.21E-01	1.96E-01
n-Butanol (C4H10O)	8.19E-02	6.04E-04	2.82E-07	6.31E-03	1.15E-02	1.44E-02	1.06E-03	1.54E-02	6.82E-03	1.09E-01	3.52E-01	2.29E-01
Nickel (II) sulfate (NiSO4)	1.52E+01	9.62E-04	4.58E-07	2.20E-01	1.10E-01	1.02E+00	3.20E-02	1.15E-01	8.81E-02	5.92E-01	7.31E+00	7.89E-01
Nitric acid (HNO3, 50%)	6.93E-02	2.06E-04	1.02E-07	3.06E-03	6.21E-03	1.40E-02	1.38E-03	4.50E-03	6.77E-04	6.33E-02	1.70E-01	3.89E-02
Nitrogen (N2)	4.80E-03	5.10E-05	2.13E-08	1.58E-03	1.19E-03	2.32E-03	1.49E-04	2.83E-03	1.72E-03	1.80E-02	7.13E-02	1.49E-02
Oxygen (O2)	1.21E-02	1.28E-04	5.37E-08	3.99E-03	2.99E-03	5.85E-03	3.75E-04	7.12E-03	4.34E-03	4.53E-02	1.80E-01	3.77E-02
Palladium (Pd)	2.57E+04	4.73E-01	3.55E-04	6.59E+02	2.73E+02	3.26E+03	9.86E+00	7.11E+01	1.21E+02	3.63E+02	3.04E+03	1.18E+03
Phenol (C6H5OH)	1.39E-01	3.02E-04	1.74E-07	9.13E-03	2.15E-02	1.73E-02	1.80E-03	2.92E-02	8.18E-03	1.58E-01	5.17E-01	3.29E-01
Phosphorus trichloride (PCl3)	1.65E-01	9.52E-04	7.91E-07	1.57E-02	1.51E-02	2.32E-02	4.38E-03	1.01E-01	2.93E-02	1.92E-01	7.80E-01	1.62E-01
Potassium hydroxide (KOH)	1.09E-01	1.91E-04	1.32E-07	6.81E-03	6.22E-03	1.22E-02	1.28E-03	2.97E-02	1.13E-02	9.97E-02	3.97E-01	8.20E-02
Potassium iodate (KIO3)	1.34E-01	5.50E-04	2.64E-07	1.64E-02	1.26E-02	2.46E-02	2.09E-03	3.41E-02	1.79E-02	2.04E-01	8.17E-01	1.59E-01

Potassium iodide (KI)	8.78E-02	-1.56E-04	8.05E-08	9.99E-04	1.57E-03	2.30E-03	6.27E-04	2.96E-02	4.47E-03	2.77E-02	1.19E-01	2.73E-02
Silica sand	9.57E-04	1.25E-05	2.32E-09	9.18E-05	1.58E-04	2.58E-04	4.66E-05	1.08E-03	6.10E-05	5.82E-03	4.10E-03	1.18E-03
Sodium (Na)	1.34E-01	3.27E-04	1.43E-07	5.59E-03	5.58E-03	1.05E-02	2.14E-03	2.08E-02	6.00E-03	8.83E-02	3.62E-01	7.15E-02
Sodium carbonate (Na2CO3)	5.19E-02	6.36E-05	2.88E-08	1.72E-03	1.83E-03	6.08E-03	5.78E-04	7.49E-03	1.22E-03	2.79E-02	1.11E-01	1.85E-02
Sodium chloride (NaCl)	5.09E-02	3.91E-05	1.80E-08	8.40E-04	7.48E-04	1.57E-03	3.40E-04	3.75E-03	8.94E-04	1.48E-02	8.00E-02	9.99E-03
Sodium hydroxide (NaOH, 50%)	7.12E-02	1.85E-04	7.45E-07	4.82E-03	3.95E-03	7.60E-03	8.78E-04	1.27E-02	5.23E-03	6.29E-02	2.66E-01	4.88E-02
Sodium methoxide (CH3ONa)	1.30E-01	4.32E-04	7.27E-07	5.39E-03	5.90E-03	1.12E-02	1.60E-03	1.84E-02	6.77E-03	8.05E-02	3.91E-01	1.12E-01
Sodium nitrite (NaNO2)	1.73E-01	5.63E-04	7.02E-07	8.12E-03	9.29E-03	1.77E-02	3.56E-03	2.52E-02	8.68E-03	1.27E-01	5.20E-01	1.20E-01
Sulfur dioxide (SO2)	5.49E-02	3.99E-04	1.87E-07	1.10E-02	5.73E-03	5.04E-02	4.64E-04	5.56E-03	1.66E-03	2.58E-02	1.55E-01	5.82E-02
Sulfuric acid (H2SO4)	3.30E-02	1.49E-04	7.08E-08	1.67E-03	1.54E-03	7.24E-03	2.20E-04	2.21E-03	3.73E-04	7.95E-03	4.92E-02	2.06E-02
Sulfuryl chloride (SO2Cl2)	1.55E-01	5.77E-04	6.52E-07	1.51E-02	9.11E-03	6.02E-02	2.14E-03	1.72E-02	6.05E-03	7.82E-02	4.07E-01	1.01E-01
tert-Butyl alcohol (C4H10O)	7.02E-02	4.26E-04	1.70E-07	6.57E-03	1.26E-02	1.99E-02	1.30E-03	1.92E-02	5.63E-03	1.21E-01	3.90E-01	2.26E-01
Tetrahydrofuran (C4H8O)	2.77E-01	1.15E-03	5.37E-07	1.72E-02	2.08E-02	3.74E-02	4.96E-03	5.21E-02	2.09E-02	2.68E-01	1.06E+00	3.07E-01
Tetramethylethylenediamine (C6H16N2, TMEDA)	3.77E-01	9.63E-04	2.23E-06	1.53E-02	1.69E-02	3.31E-02	3.92E-02	5.19E-02	1.59E-02	2.58E-01	1.03E+00	3.10E-01
Tin (Sn)	1.49E+03	8.65E-02	1.55E-06	3.31E-01	1.98E-01	4.89E-01	8.19E-03	1.31E+00	7.27E-02	7.41E+00	3.93E+00	6.98E+01
Titanium dioxide (TiO2)	2.30E-01	1.72E-03	7.61E-07	1.98E-02	2.91E-02	4.11E-02	4.33E-03	1.13E-01	7.90E-02	3.28E-01	1.12E+00	2.52E-01
Titanium tetrachloride (TiCl4)	1.27E-01	9.23E-04	6.41E-07	7.41E-03	1.41E-02	1.55E-02	2.28E-03	6.23E-02	3.21E-02	1.27E-01	4.78E-01	1.07E-01
Toluene (C7H8)	7.43E-04	-1.52E-07	4.16E-10	1.18E-03	4.37E-03	3.75E-03	2.26E-04	7.70E-05	2.15E-04	3.54E-02	5.13E-02	1.77E-01
Treatment of wastewater	1.75E-01	1.82E-04	1.84E-07	5.06E-03	5.95E-03	1.04E-02	1.38E-03	2.34E-02	1.06E-02	1.01E-01	3.07E-01	5.50E-02
Trimethyl borate (C3H9BO3)	1.68E-01	7.40E-04	3.01E-07	6.93E-03	8.25E-03	1.62E-02	1.42E-03	2.40E-02	5.26E-03	5.70E-02	3.93E-01	1.47E-01
Urea (CH4N2O)	1.98E-01	9.40E-04	4.42E-07	7.92E-03	6.93E-03	2.54E-02	5.34E-03	1.60E-02	3.84E-03	1.22E-01	4.69E-01	1.76E-01
Xylene (C8H10)	8.31E-04	-2.45E-07	4.76E-10	1.38E-03	4.80E-03	4.46E-03	9.61E-04	9.86E-05	2.55E-04	3.94E-02	5.76E-02	1.82E-01
Zinc (Zn)	2.73E+00	6.98E-04	2.01E-07	1.98E-02	2.48E-02	5.27E-02	6.91E-02	5.59E-02	7.23E-02	3.19E-01	2.98E+00	2.70E-01

Supplementary Table 42. Characterization factors for emissions to air extracted from Ecoinvent database (Part I).

item	value	unit	IPCC 2013 (kg CO_2-eq)	cumulative energy demand (MJ-eq)	ReCiPe Midpoint (E)								
					agricultural land occupation	climate change	fossil depletion	freshwater ecotoxicity	freshwater eutrophication	human toxicity	ionising radiation	marine ecotoxicity	marine eutrophication
CO2	**1**	**kg**	1.00E+00	0.00E+00	0.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NOx	**1**	**kg**	-7.71E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.90E-02
Butane	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
N2	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ar	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E-05	0.00E+00	1.44E-02	0.00E+00	1.79E-05	0.00E+00
SO2	**1**	**kg**	-3.84E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CH4	**1**	**kg**	2.80E+01	0.00E+00	0.00E+00	7.60E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Particulate	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
HF	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.66E+02	0.00E+00	0.00E+00	0.00E+00
Pb	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.70E-01	0.00E+00	2.31E+04	0.00E+00	2.94E+02	0.00E+00
As	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.68E+00	0.00E+00	5.53E+05	0.00E+00	1.89E+04	0.00E+00
Ni	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.29E+01	0.00E+00	6.81E+02	0.00E+00	1.29E+05	0.00E+00
H2	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Isopropanol	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Acetone	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.83E-05	0.00E+00	1.49E-01	0.00E+00	7.46E-05	0.00E+00
Acetic anhydride	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.52E-06	0.00E+00	0.00E+00	0.00E+00	3.21E-07	0.00E+00
2-Methoxyethanol	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.56E-08	0.00E+00	2.35E+00	0.00E+00	1.02E-06	0.00E+00
Dimethylformamide	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Toluene	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.18E-05	0.00E+00	8.20E-01	0.00E+00	9.07E-05	0.00E+00
Acetonitrile	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.70E-04	0.00E+00	4.71E-01	0.00E+00	1.74E-03	0.00E+00
4-tert-butylpyridine	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.24E-04	0.00E+00	0.00E+00	0.00E+00	8.25E-03	0.00E+00
Au	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.93E+01	0.00E+00	2.59E+06	0.00E+00	1.47E+06	0.00E+00
Ethylene glycol	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-04	0.00E+00	2.14E-01	0.00E+00	1.63E-05	0.00E+00
Ethylenediamine	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.06E-03	0.00E+00	0.00E+00	0.00E+00	2.72E-04	0.00E+00
Monochlorobenzene	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.49E-04	0.00E+00	1.88E+00	0.00E+00	3.94E-02	0.00E+00
Al	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TiO2	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
DMSO	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cu	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.01E+01	0.00E+00	5.21E+01	0.00E+00	9.15E+04	0.00E+00

Supplementary Table 43. Characterization factors for emissions to air extracted from Ecoinvent database (Part II).

item	ReCiPe Midpoint (E)									ReCiPe Endpoint (E,A)		
	metal depletion	natural land transformation	ozone depletion	particulate matter formation	photochemical oxidant formation	terrestrial acidification	terrestrial ecotoxicity	urban land occupation	water depletion	ecosystem quality	human health	resources
CO2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.72E-02	3.42E-02	0.00E+00
NOx	0.00E+00	0.00E+00	0.00E+00	2.20E-01	1.00E+00	7.10E-01	0.00E+00	0.00E+00	0.00E+00	1.47E-02	5.58E-01	0.00E+00
Butane	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.95E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.26E-04	0.00E+00
N2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ar	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.74E-01	0.00E+00	3.72E-05	0.00E+00	0.00E+00	8.16E-06	3.55E-04	0.00E+00
SO2	0.00E+00	0.00E+00	0.00E+00	2.00E-01	8.11E-02	1.00E+00	0.00E+00	0.00E+00	0.00E+00	2.07E-02	8.93E-01	0.00E+00
CH4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.07E-01	2.60E-01	0.00E+00
Particulate	0.00E+00	0.00E+00	0.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.54E+00	0.00E+00
HF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.82E+00	0.00E+00
Pb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.80E+00	0.00E+00	0.00E+00	2.00E+00	1.58E+02	0.00E+00
As	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+01	0.00E+00	0.00E+00	7.27E+00	3.78E+03	0.00E+00
Ni	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.00E+01	0.00E+00	0.00E+00	5.07E+01	4.65E+00	0.00E+00
H2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Isopropanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.18E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.21E-04	0.00E+00
Acetone	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.59E-01	0.00E+00	3.03E-05	0.00E+00	0.00E+00	6.69E-06	1.08E-03	0.00E+00
Acetic anhydride	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.30E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-Methoxyethanol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E-07	0.00E+00	0.00E+00	0.00E+00	2.48E-04	0.00E+00
Dimethylformamide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Toluene	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E+00	0.00E+00	1.35E-05	0.00E+00	0.00E+00	3.00E-06	6.01E-03	0.00E+00
Acetonitrile	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.70E-04	0.00E+00	0.00E+00	8.18E-05	3.22E-03	0.00E+00
4-tert-butylpyridine	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.29E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Au	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.46E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethylene glycol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.30E-01	0.00E+00	3.13E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethylenediamine	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Monochlorobenzene	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.13E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Al	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TiO2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
DMSO	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.20E+02	0.00E+00	0.00E+00	1.16E+02	3.56E-01	0.00E+00

Supplementary Table 44. Characterization factors for emissions to water extracted from Ecoinvent database (Part I).

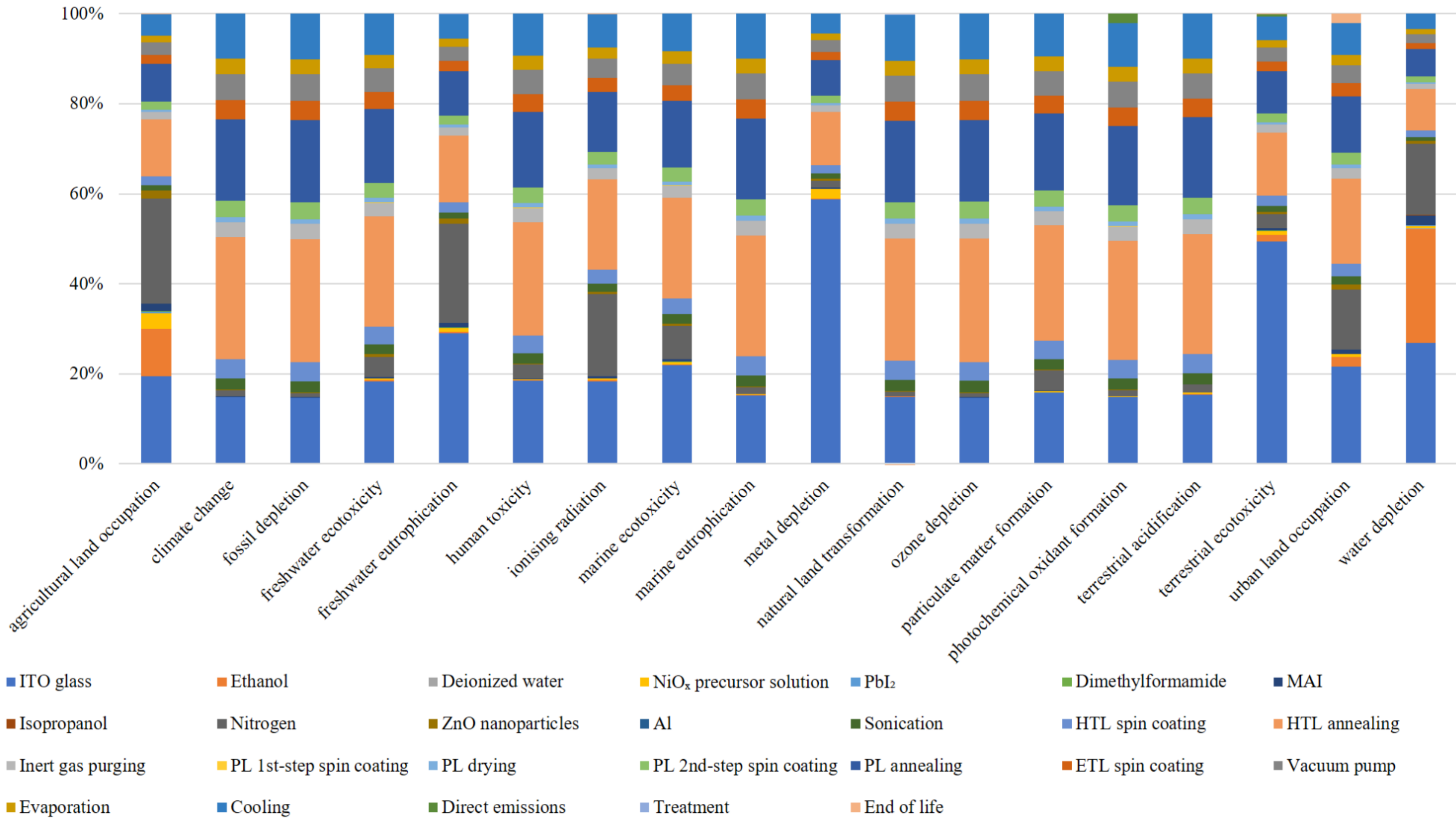
item	value	unit	IPCC 2013 (kg CO_2-eq)	cumulative energy demand (MJ-eq)	ReCiPe Midpoint (E)								
					agricultural land occupation	climate change	fossil depletion	freshwater ecotoxicity	freshwater eutrophication	human toxicity	ionising radiation	marine ecotoxicity	marine eutrophication
Chloride	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
COD	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.79E-01	0.00E+00	0.00E+00	0.00E+00	3.25E-03	0.00E+00
Sulfate	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Susp. Solids	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Fluoride	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mineral oil	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ammonia	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00
Boric acid	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Barium	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.69E+00	0.00E+00	6.63E+04	0.00E+00	1.54E+04	0.00E+00
Phenol	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.60E-02	0.00E+00	1.13E-02	0.00E+00	3.58E-05	0.00E+00
Chromium, Copper, tin, lead, Nickel, zinc	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.02E-01	0.00E+00	2.05E-03	0.00E+00	1.20E+02	0.00E+00
Arsenic, antimony	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.54E+01	0.00E+00	3.11E+04	0.00E+00	3.24E+04	0.00E+00
Cadmium	**1**	**kg**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.05E+00	0.00E+00	5.52E+02	0.00E+00	1.49E+03	0.00E+00

Supplementary Table 45. Characterization factors for emissions to water extracted from Ecoinvent database (Part II).

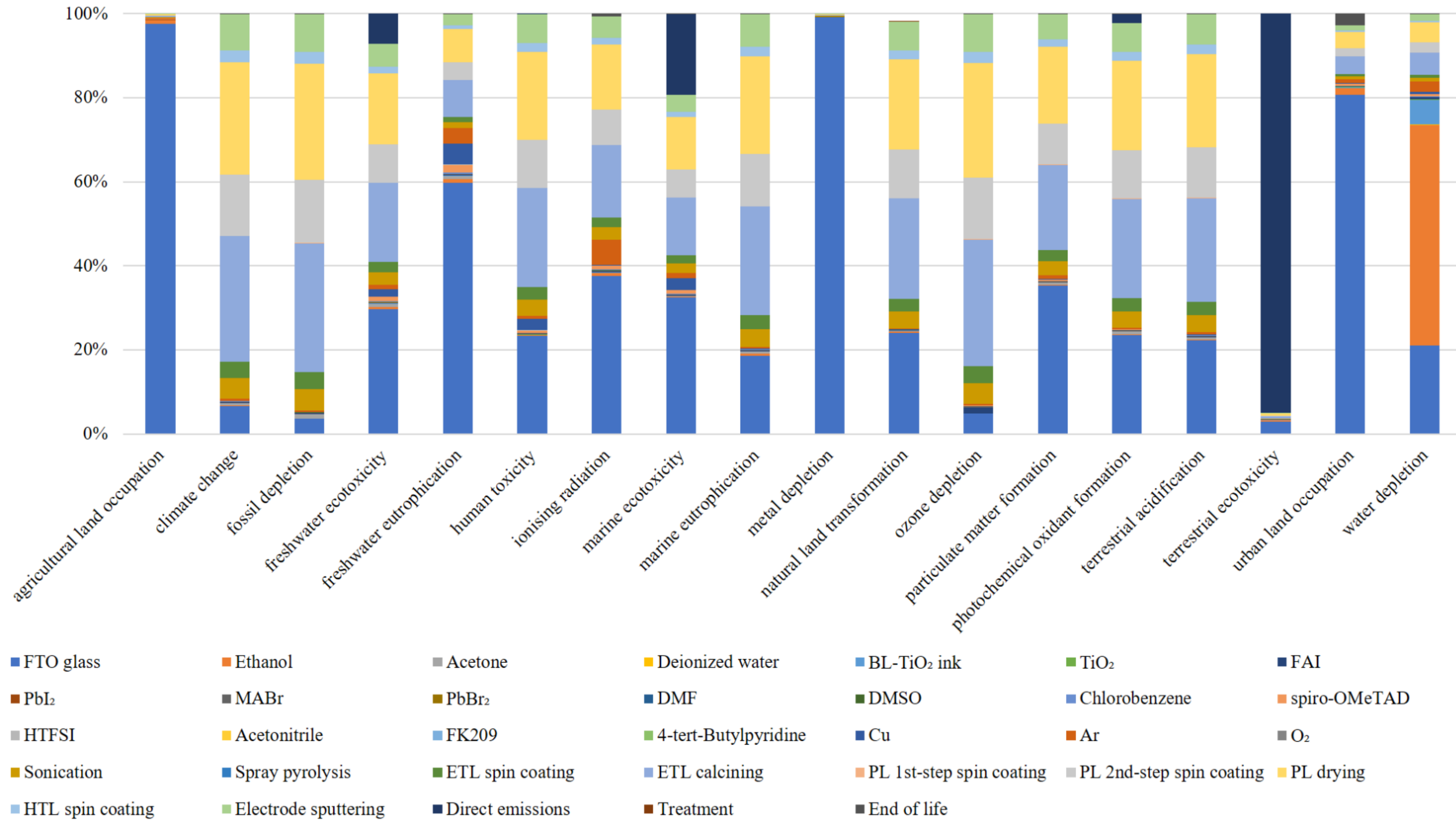
item	ReCiPe Midpoint (E)									ReCiPe Endpoint (E,A)		
	metal depletion	natural land transformation	ozone depletion	particulate matter formation	photochemical oxidant formation	terrestrial acidification	terrestrial ecotoxicity	urban land occupation	water depletion	ecosystem quality	human health	resources
Chloride	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
COD	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.16E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sulfate	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Susp. Solids	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Fluoride	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mineral oil	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ammonia	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Boric acid	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Barium	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.56E-18	0.00E+00	0.00E+00	3.95E+00	0.00E+00	0.00E+00
Phenol	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.69E-05	0.00E+00	0.00E+00	7.39E-05	7.72E-05	0.00E+00
Chromium, Copper, tin, lead, Nickel, zinc	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.46E-20	0.00E+00	0.00E+00	3.20E-02	8.21E-03	0.00E+00
Arsenic, antimony	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.58E-18	0.00E+00	0.00E+00	8.33E+00	2.12E+02	0.00E+00
Cadmium	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.46E-19	0.00E+00	0.00E+00	3.93E-01	3.77E+00	0.00E+00

S6. Environmental profiles of the metal oxide module, mixed-cation module, SnO_2 module, and semi-transparent module

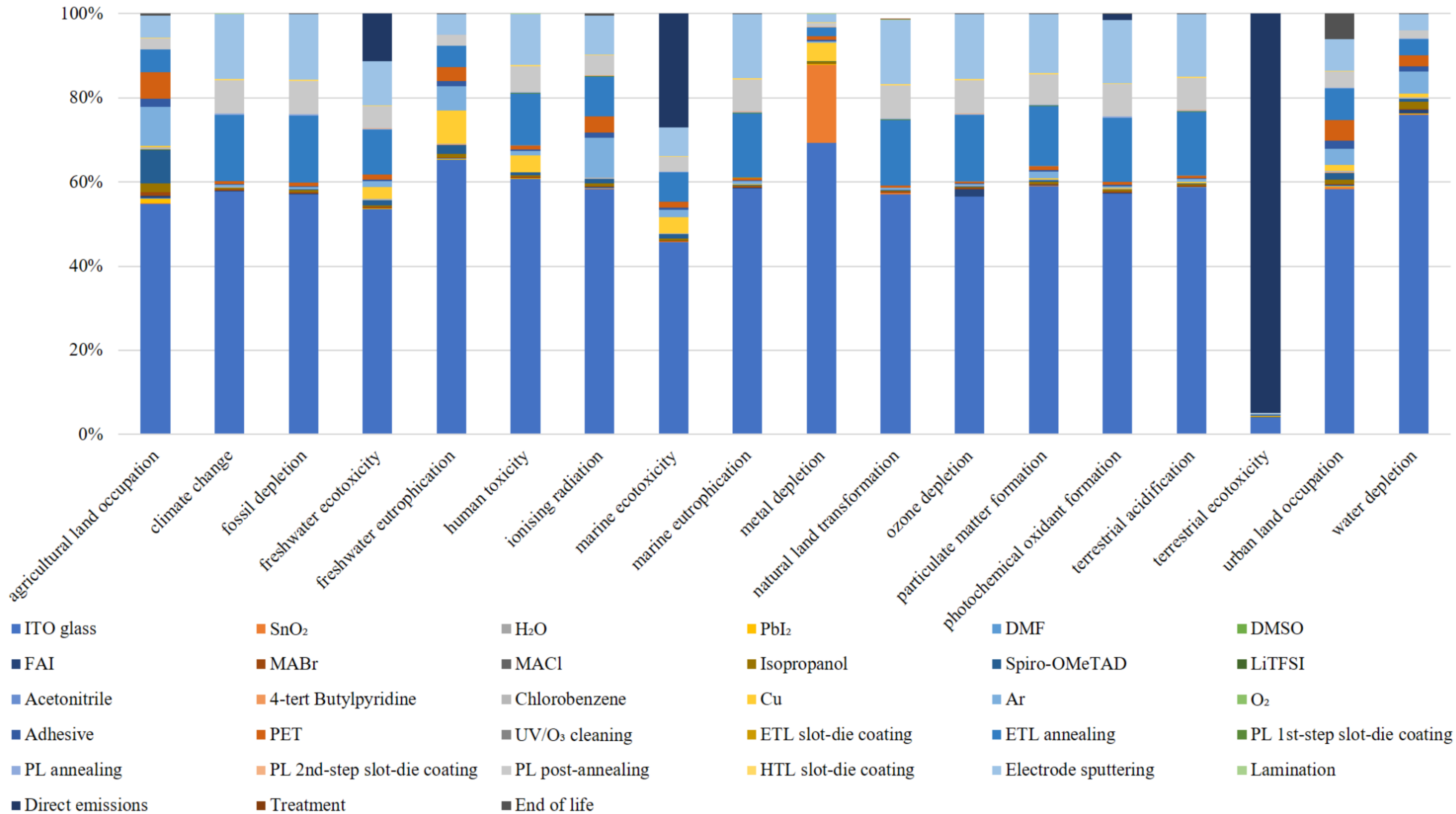
The environmental profiles of the metal oxide module, mixed-cation module, SnO_2 module, and semi-transparent module in terms of 21 impact categories are shown in Supplementary Figure 5 to Supplementary Figure 8.



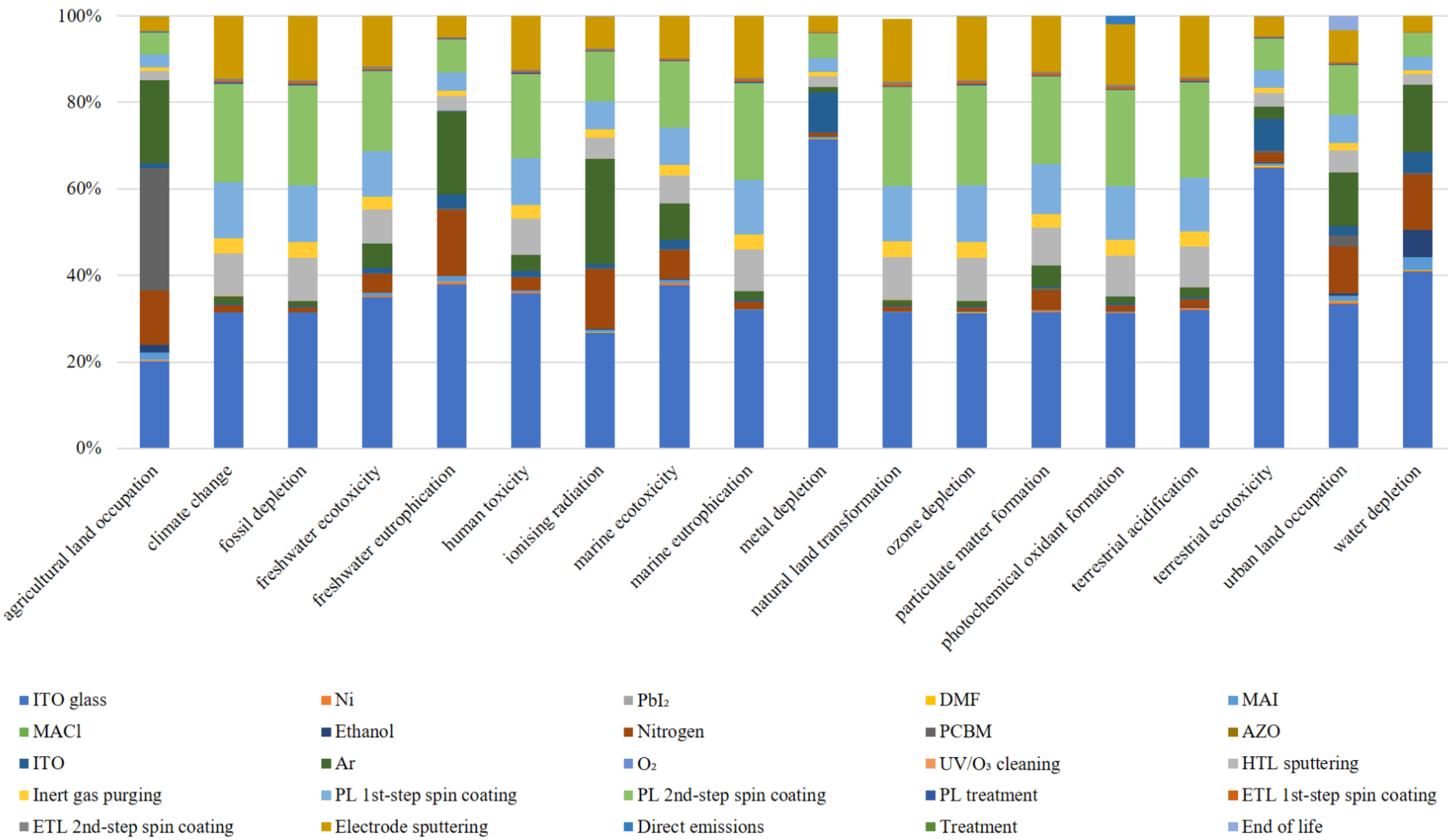
Supplementary Figure 5. Environmental profile of 1 m^2 of the metal oxide module.



Supplementary Figure 6. Environmental profile of 1 m^2 of the mixed-cation module.

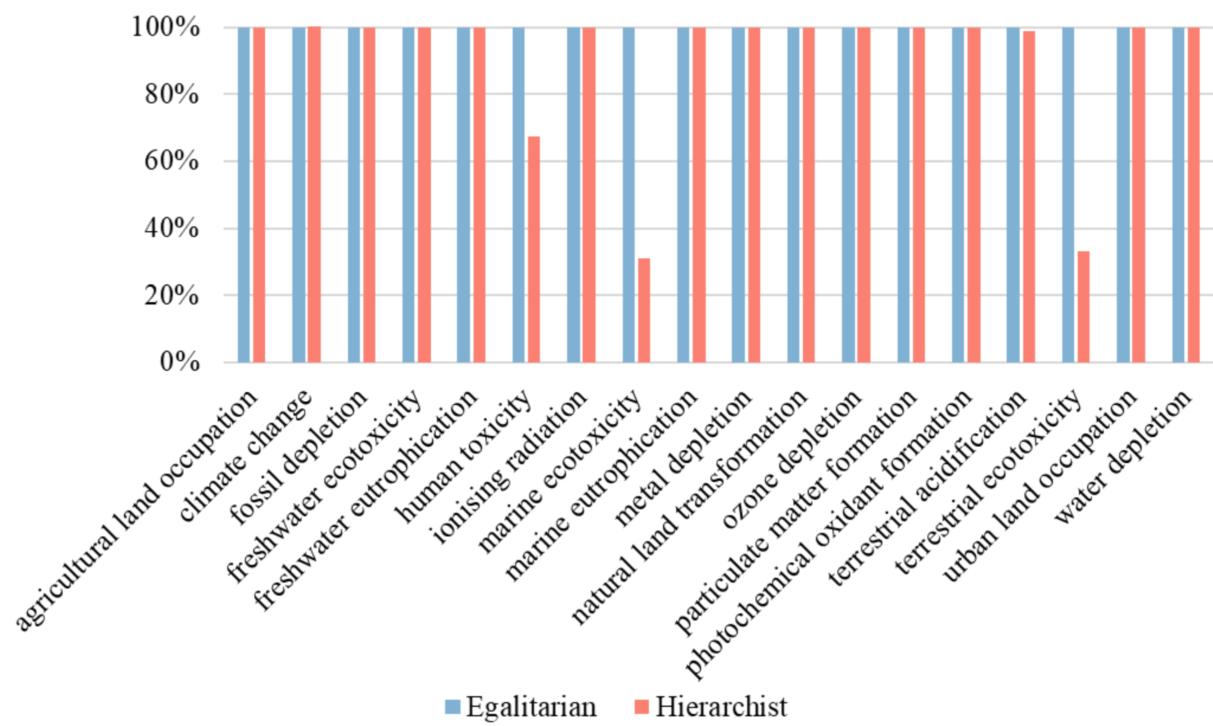


Supplementary Figure 7. Environmental profile of 1 m^2 of the SnO_2 module.



Supplementary Figure 8. Environmental profile of 1 m^2 of the semi-transparent module.

In this work, the Egalitarian perspective is selected for the LCIA method following the selection in previous LCA studies on PCSs.[1,22] To highlight the difference between the Egalitarian and Hierarchist perspectives, one example regarding the metal oxide module is presented below. We note that for most of the midpoint indicators, the results are the same for the Egalitarian and Hierarchist perspectives. However, the results regarding human toxicity, marine ecotoxicity, and terrestrial ecotoxicity using Hierarchist perspective are substantially lower than those using Egalitarian perspective by 33%, 69%, and 67%, respectively, due to the longer time frame and a broader range of impact categories for the Egalitarian perspective.



Supplementary Figure 9. Comparison of the LCIA results between the Egalitarian and Hierarchist perspectives for the metal oxide module.

S7. Primary energy consumption and global warming potential

EPBT is an important metric for PV systems, which is defined as the time needed to generate as much energy as was consumed during manufacturing and operations of the system.[23] There is little energy consumption during the operation phase of perovskite PV modules, so EPBT is dominated by the energy embedded in raw materials, as well as the energy consumption during production and recycling processes. The GHG emission factor is obtained by dividing the life cycle GHG emissions by the total electric energy production during the lifetime of the given PSC system. When calculating the EPBT and GHG emission factor, we account for the individual difference of PSCs and impacts of operating conditions on module performance and consider the fluctuation of parameters such as annual irradiation, module efficiency, performance ratio, lifetime, primary consumption, and global warming potential.

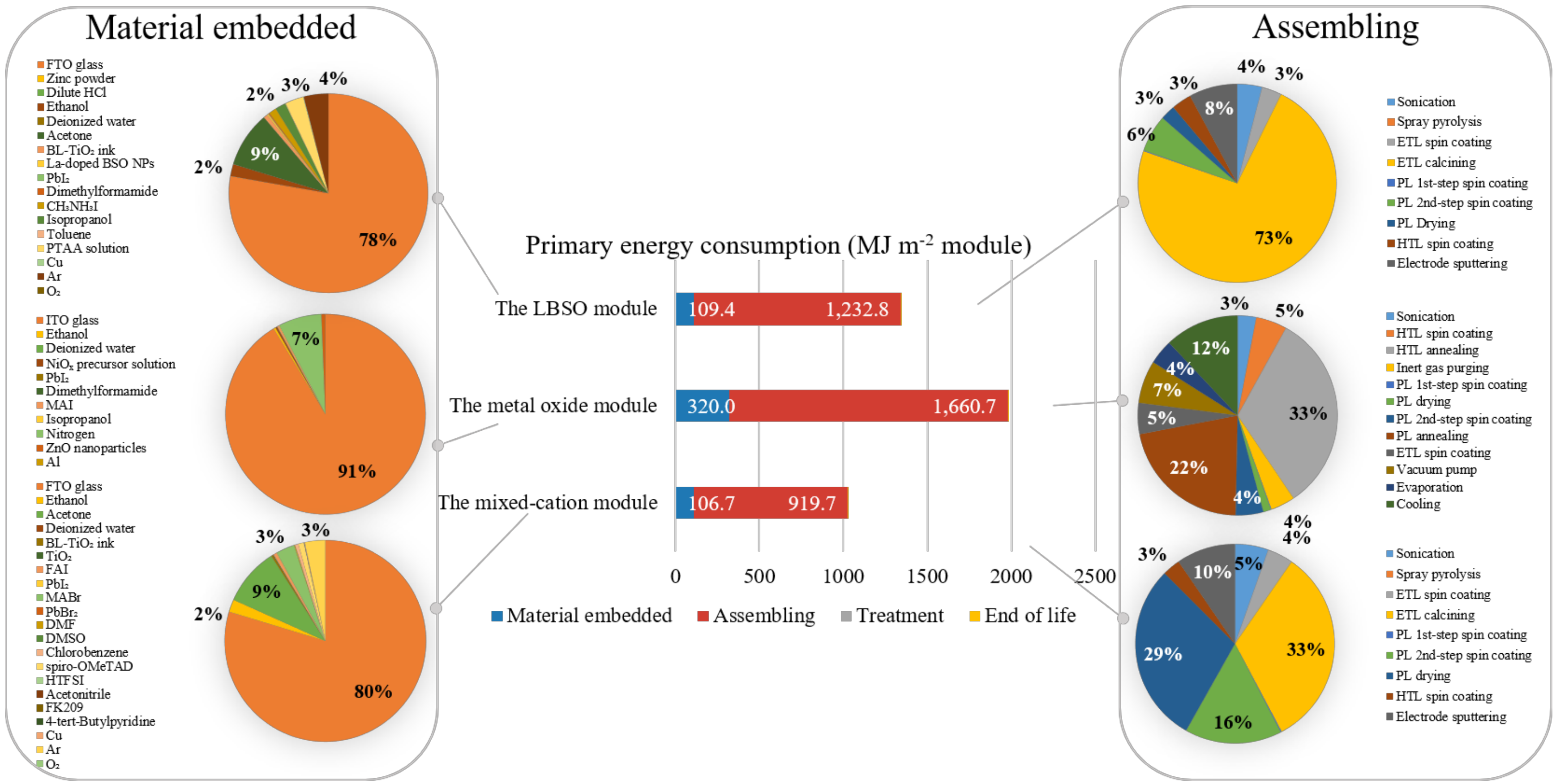
As shown in Supplementary Figure 10, during the lifetime of the first three perovskite PV modules, the metal oxide module presents the highest primary energy consumption of up to 1980.9 MJ/m^2-module, and the mixed-cation module has the lowest primary energy consumption of 1027.3 MJ/m^2-module. For all investigated modules, the energy consumed during manufacturing accounts for 39.8% to 91.8% of the total primary energy consumption, while energy consumption during the treatment phase and the end of life is negligible. Moreover, the breakdowns of the energy embedded in raw materials and energy consumed during module assembly vary significantly from module to module.

For both the LBSO and mixed-cation modules, the embedded energy is dominated by FTO glass, while ITO glass is the major contributor in the metal oxide module due to the use of energy-intensive indium. FTO glass contributes 78% and 80% of the total primary energy consumption of the LBSO module and the mixed-cation module, respectively. FTO glass accounts for a large proportion of the total primary energy consumption, mainly because it makes up over 90% of the total module mass. The dominance of ITO glass in these metrics is fundamentally due to the use of precious metals, which consumes extremely large amounts of energy in smelting the metal ores, despite the small total mass used. Herein, we note that the use of precious metals and substrates are two significant environmental hotspots, which is consistent with the results reported in the literature.[1] New materials and device architectures can be devised by reducing the consumption of these hotspot materials, which is likely to result in much lower primary energy consumption and global warming potential.

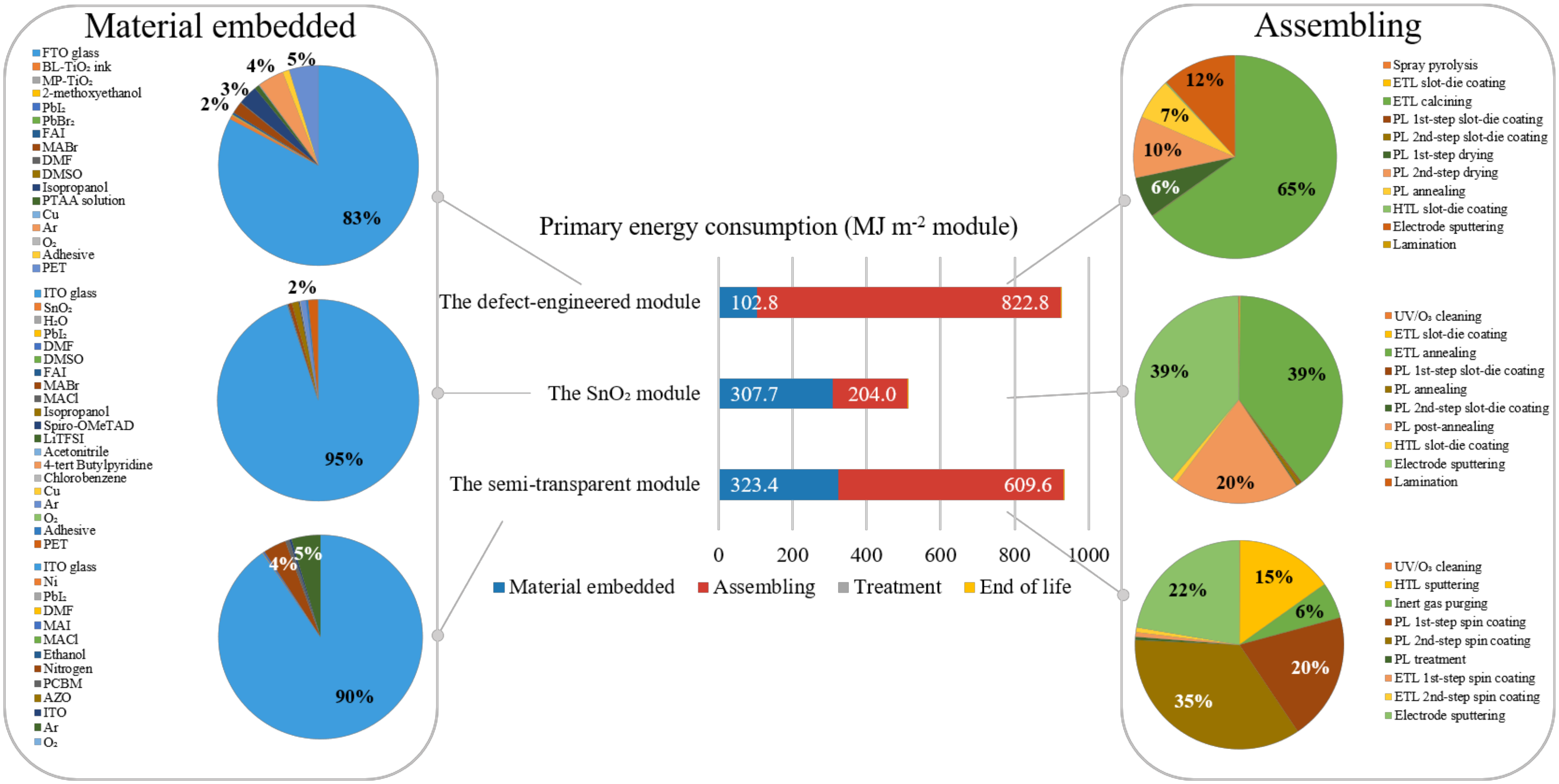
Regarding the module assembly phase, the heating processes, including annealing, calcining, and other drying processes, are always the most energy-intensive aspects. Specifically, the heating processes account for 76%, 56%, and 62% of the total primary energy consumption of the fabrication of the LBSO, metal oxide, and mixed-cation modules, respectively. Spin coating and electrode deposition are the other major contributors besides the heating processes. The overall energy consumption will be brought down further by adopting metal oxide layers that are compatible with crystallization processes at even lower temperatures, for fabricating scaled PSC modules in the future.

Supplementary Figure 12 depicts the detailed breakdowns of global warming potential during the lifetime of the first three perovskite PV modules. Distinct from primary energy consumption, there are five contributing phases to the total global warming potential, i.e., material embedded, module assembly, direct emissions, treatment, and end of life. Similar to the results of primary energy consumption, FTO glass, ITO glass, and heating processes are the major contributors. We notice that the global warming potential distribution of the module assembling phase is exactly the same as the primary energy distribution for each module because electricity is the only input during module assembling.

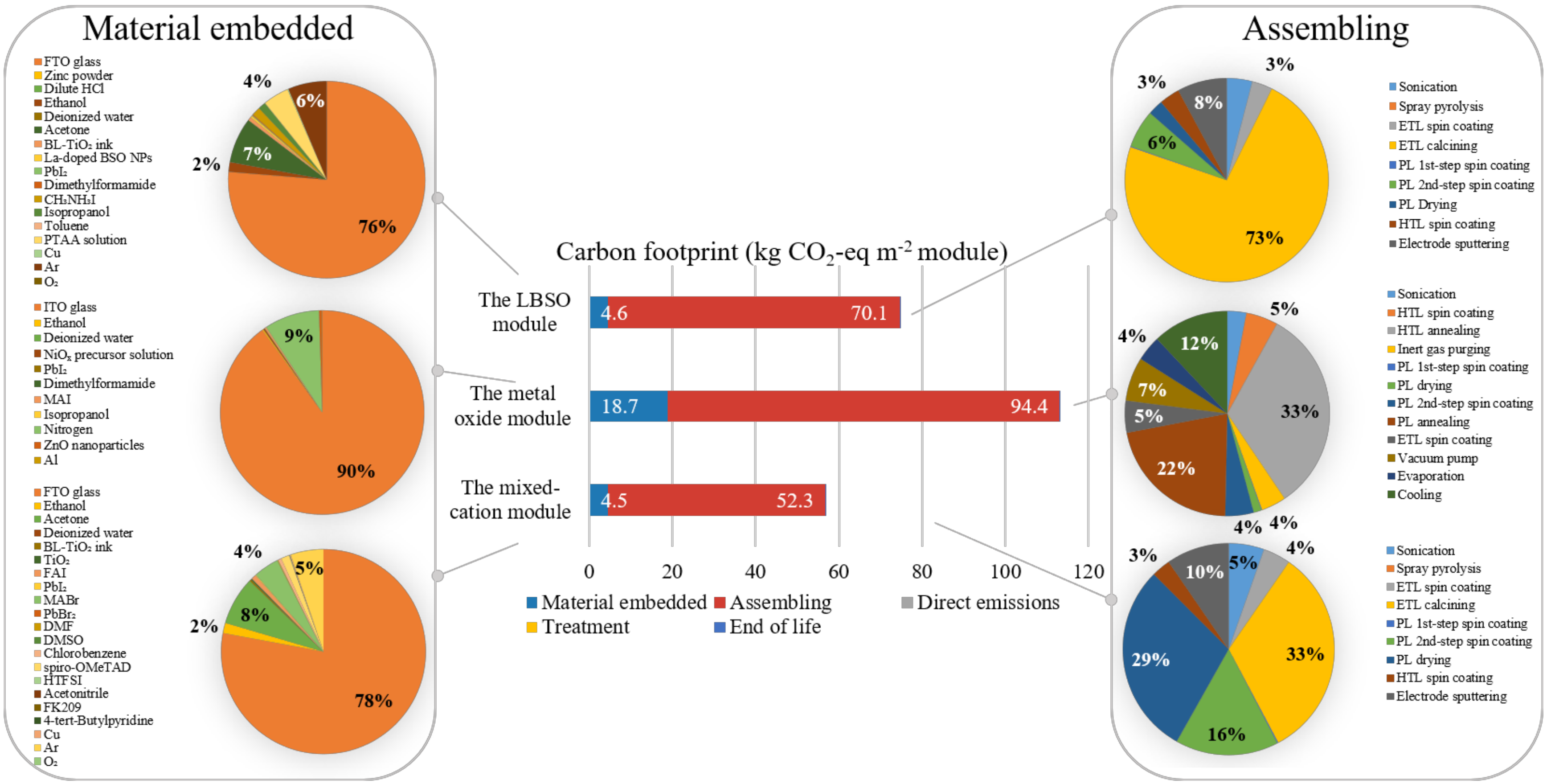
The comparative results of primary energy consumption and global warming potential among the remaining PSCs are given in Supplementary Figure 11 and Supplementary Figure 13, respectively. For the primary energy consumption and global warming potential embedded in the raw materials, the use of substrate and thermal treatment are still the major contributors. We note that the environmental impact of the metal oxide module is generally the highest, presumably due to the involvement of energy-intensive heat processes with much longer treatment time and higher temperature than the remaining PSC fabrication steps, such as annealing and calcining.[4] Moreover, the estimation of the metal oxide module based on laboratory-scale data is likely to provide conservative insights and serve as the upper bound on impacts for all impact categories.



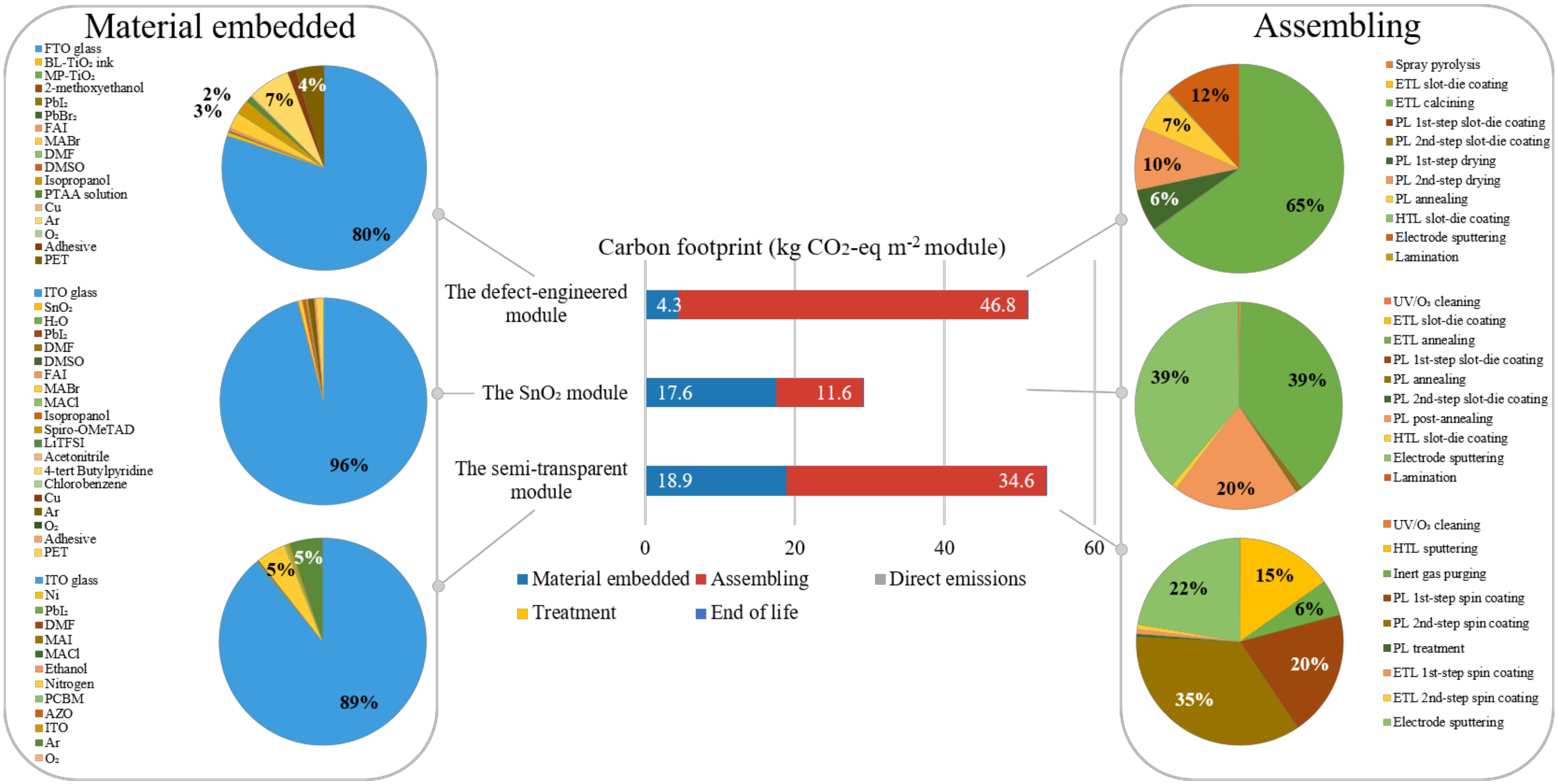
Supplementary Figure 10. Profile of primary energy consumption of the LBSO, metal oxide, and mixed-cation modules (The bar charts in the middle reflect the breakdown of primary energy consumption during different phases ending up with landfill. The pie charts on the left reveal the energy embedded in various feedstocks for the three PSCs, while the pie charts on the right depict the energy consumption of different manipulations during the assembling phase for the three PSCs).



Supplementary Figure 11. Profile of primary energy consumption of the defect-engineered, SnO_2, and semi-transparent modules (The bar charts in the middle reflect the breakdown of primary energy consumption during different phases ending up with landfill. The pie charts on the left reveal the energy embedded in various feedstocks for the three PSCs, while the pie charts on the right depict the energy consumption of different manipulations during the assembling phase for the three PSCs).



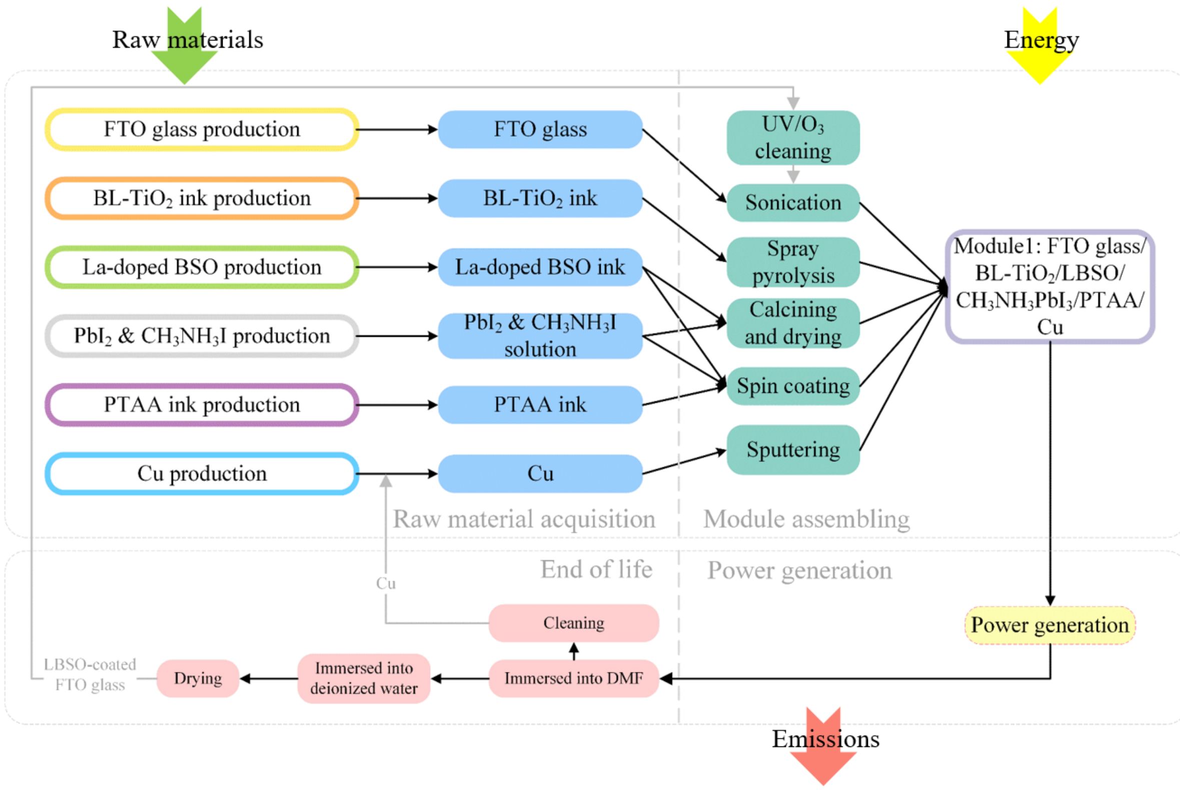
Supplementary Figure 12. Profile of global warming potential of the LBSO, metal oxide, and mixed-cation modules (The bar charts in the middle reflect the breakdown of global warming potential during different phases ending up with landfill. The pie charts on the left reveal the GHG emissions embedded in various feedstocks for the three PSCs, while the pie charts on the right depict the global warming potential of different manipulations during the assembling phase for the three PSCs).



Supplementary Figure 13. Profile of global warming potential of the defect-engineered, SnO_2, and semi-transparent modules (The bar charts in the middle reflect the breakdown of global warming potential during different phases ending up with landfill. The pie charts on the left reveal the GHG emissions embedded in various feedstocks for the three PSCs, while the pie charts on the right depict the global warming potential of different manipulations during the assembling phase for the three PSCs).

S8. The role of PSC recycling

From the LCA results, one environmental hotspot facet lies in the use of FTO and ITO glass. It is therefore vital to consider PSC recycling, provided that the hotspot materials can be refurbished at relatively lower emissions and energy intensity than PSC manufacturing using virgin feedstocks. Another environmental hotspot is the use of energy-intensive heating processes, such as annealing and calcining. Many of these processes are unavoidable and would not be able to be engineered around in the short term. Therefore, it is critical to pursue recycling for PSC production. PSC recycling is also favorable for the reduction of solid waste especially given the scarcity of some materials,[24] such as indium, for the potential widespread PSC future deployment scenario. One important measurement of the environmental viability of PSC fabrication is the difference in environmental performance between the cases with and without recycling. If the environmental performance of the recycling scenario is identical or very close to that of the case without recycling, a "breakeven" point is attained, which indicates that the investigated device architecture is sufficiently cheap or more advanced recycling approaches need to be explored.

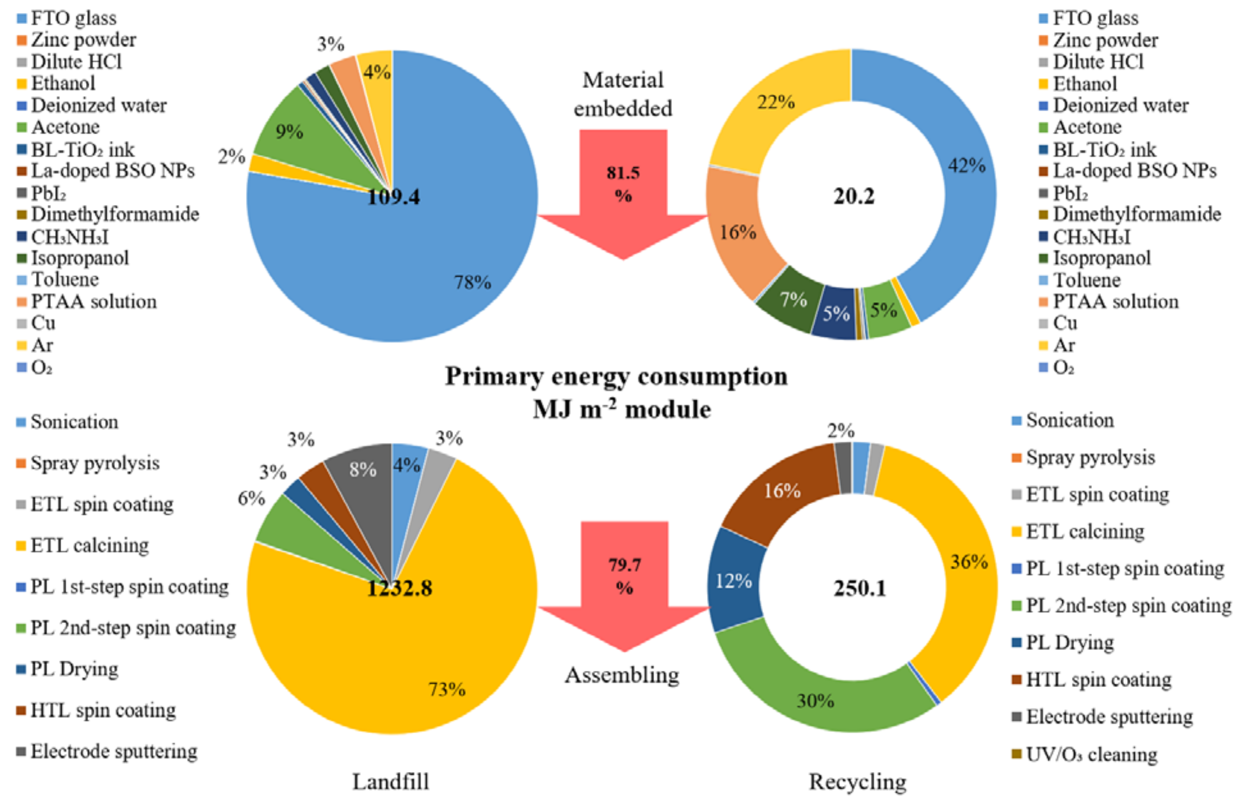


Supplementary Figure 14. The system boundary of manufacturing LBSO perovskite solar modules with recycling as the end-of-life scenario.

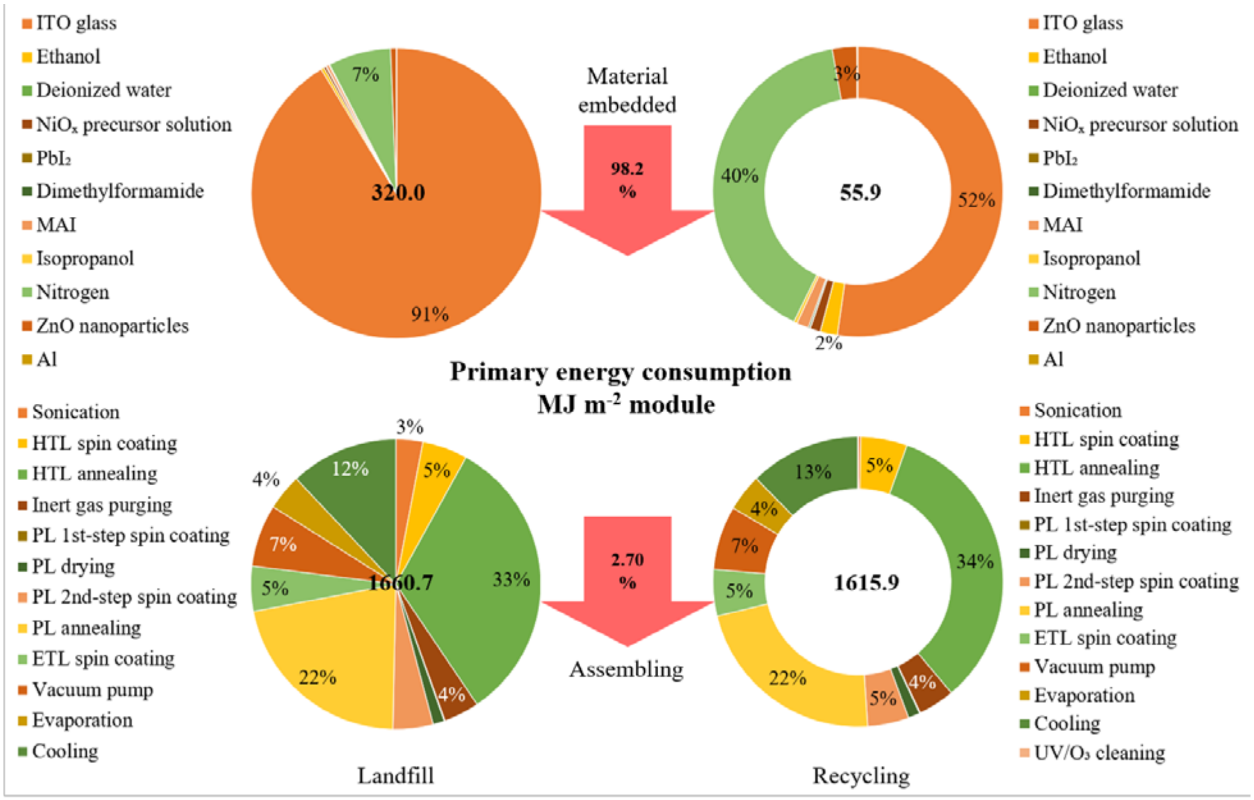
By switching the end-of-life scenario into its recycling counterpart, the system boundary is revised correspondingly, which is illustrated in Supplementary Figure 14 for the LBSO modules. The recycling of PSCs is modeled based on the avoided burden approach, where the materials potentially being reused by future generations substitute a portion of the primary counterpart. In contrast to the intensive energy use and environmental impacts in the landfill scenario, significant melioration can be foreseen in both primary energy consumption and environmental profile if the hotspot materials are carefully recovered and reused for manufacturing PSCs. Compared with the recycling approaches for commercialized PV technologies, strategies for refurbishing perovskite PV modules are much more straightforward. One of the widely reported recycling strategies for perovskite cells is to selectively dissolve the panel layers with suitable solvents.[25-27] The substrates are usually recovered and reused directly, instead of being smashed before reusing.[25-27] Metal electrodes can also be directly retrieved after cleaning if they are chemically stable and insoluble in the chosen solvent. According to the avoided burden approach, the fraction of metal or substrates recycled after the use phase of PSCs determines the amount of primary metal or substrate feedstocks that can be potentially avoided.[28] In this way, the resulting energy consumption and environmental impacts of PSC manufacturing can be significantly reduced.

Supplementary Figure 15, Supplementary Figure 16, and Supplementary Figure 17 show the changes in primary energy consumption during the material acquisition and assembling phases of three perovskite PV modules due to the recycling of hotspot module components. The results of the remaining three modules are given in the next section. The pie charts on the left depict the primary energy consumption profile considering landfill as the end-of-life scenario, while the right-hand-side donut charts refer to the recycling counterpart.

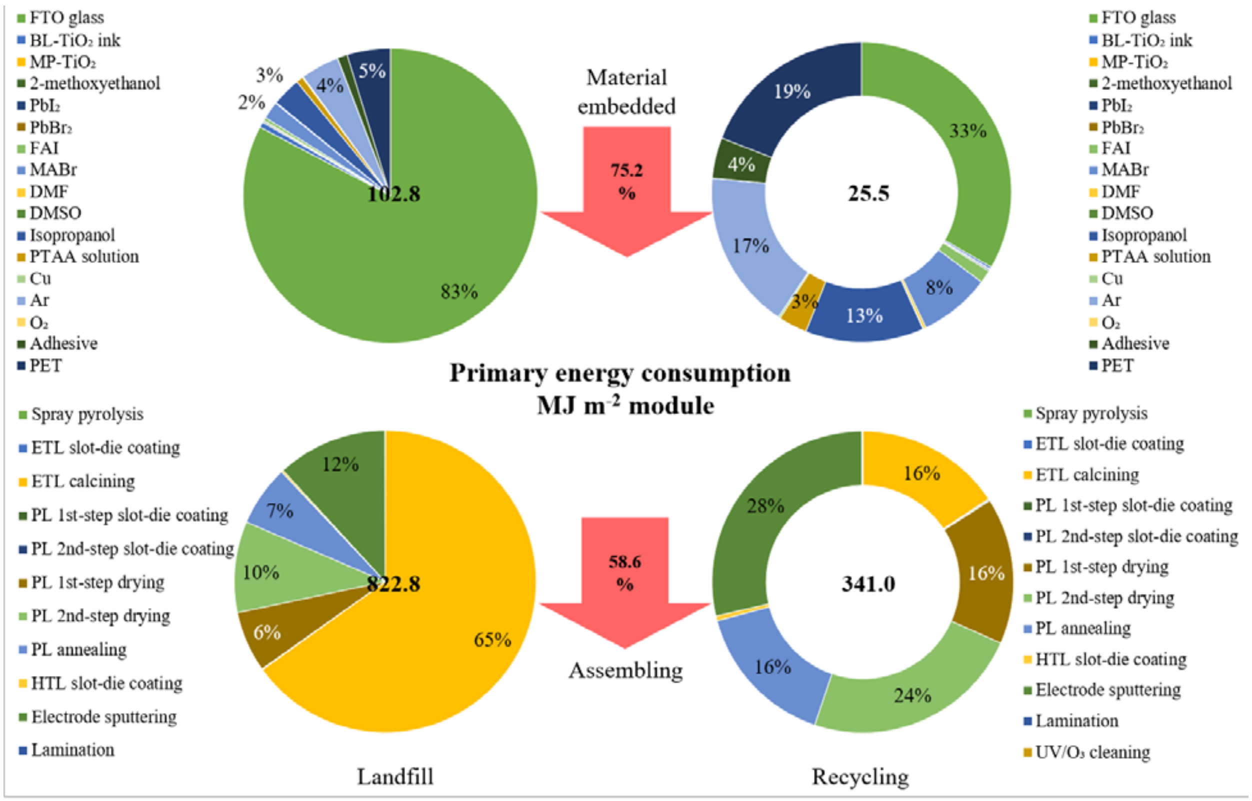
As shown in Supplementary Figure 15, by considering recycling as the end-of-life scenario of the LBSO module, the energy embedded within the raw materials is significantly reduced from 109.4 MJ/m^2-module to 20.2 MJ/m^2-module, accounting for about 81.5% of the primary energy consumption in the landfill scenario. The reasons are that the amount of copper use is reduced in the recycling scenario, and the FTO glass is assumed to be recycled and can be reused after surface treatment.[26,27] Since the blocking layer (BL) and ETL are closely attached to the FTO substrate, these layers are recovered along with the substrate. The spray pyrolysis for depositing BL-TiO_2 layer onto the substrate as well as the spin coating and calcining of ETL is also excluded to produce the LBSO module from recycled materials. Energy consumption induced by the newly introduced UV/O_3 cleaning process is relatively small compared with those of the aforementioned manipulations, so the overall primary energy consumption during the assembling phase decreases significantly by 79.7%. Both the LBSO module and defect-engineered module use FTO glass and gold and thus the effectiveness of recycling is similar, as shown in Supplementary Figure 15 and Supplementary Figure 17.



Supplementary Figure 15. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the LBSO module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).



Supplementary Figure 16. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the metal oxide module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).



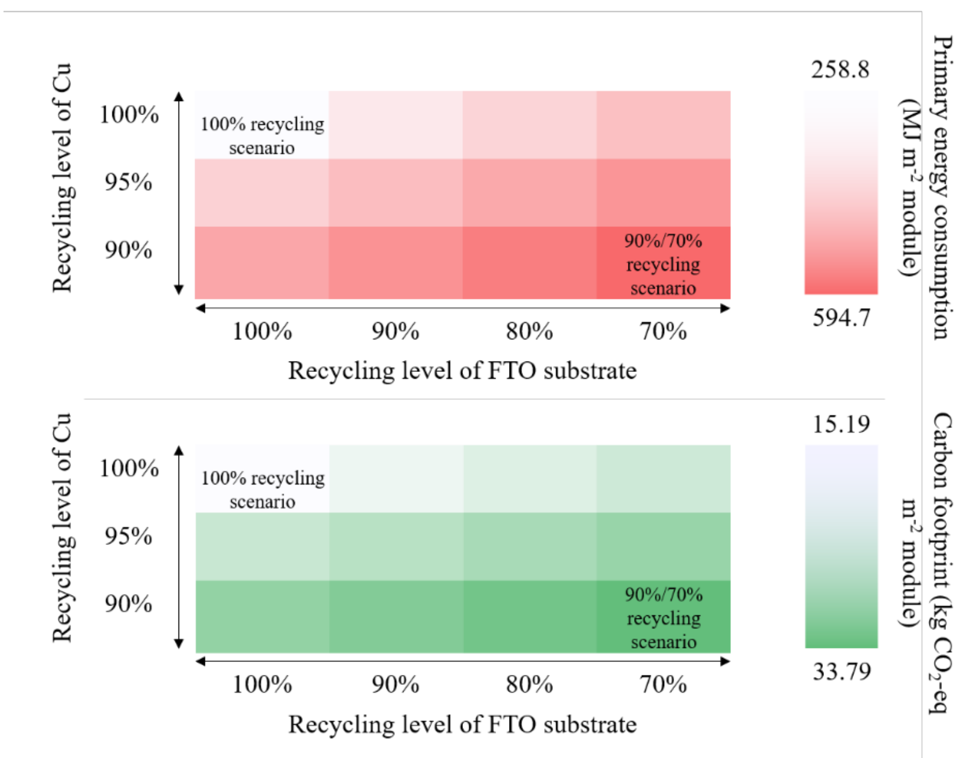
Supplementary Figure 17. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the defect-engineered module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).

As shown in Supplementary Figure 16, the metal oxide module demonstrates a totally different outcome for the recycling scenario. The ITO substrate is the only recycled material recovered via immersion in aqueous NaOH, with all other layers dissolved into the solution. Regarding primary energy embedded in raw materials, 98.2% of the primary energy consumption is eliminated by simply recycling and reusing ITO glass. The energy consumption in the assembling phase only demonstrates a slight decrease of around 2.70%. We note that such recycling methods only focus on the recycling of ITO glass, with all other active layers sacrificed and wasted. There is a critical need to develop alternative recycling strategies for more extensive material recovery and minimization of environmental consequences; it is likely such recycling strategies will be further developed and optimized as the ultimate scaled module compositions take form.

From the results of primary energy consumption change ascertained by considering recycling as the end-of-life scenario, we notice that tremendous energy saving can be achieved (even over 90% of the energy embedded in raw materials) by recovering and reusing the hotspot materials of perovskite PV modules. Meanwhile, the influence on the assembling phase cannot be ignored, considering that the assembling phase contributes to over 90% of the total primary energy consumption.

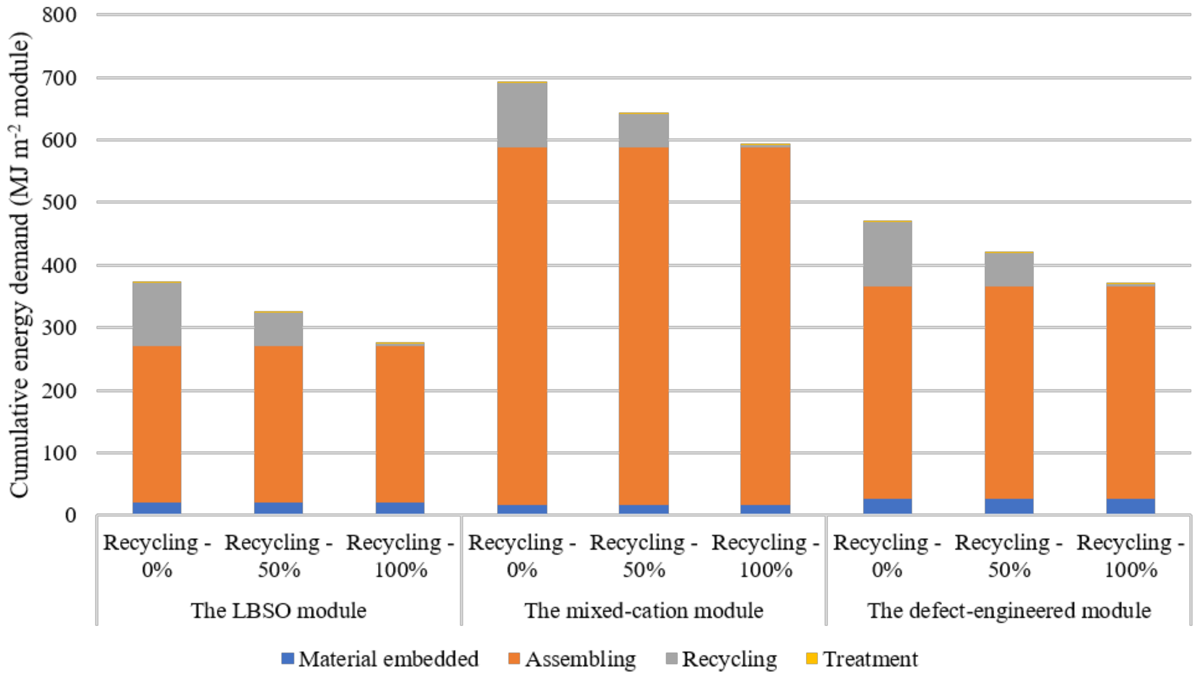
The aforementioned results hold given recycling at a nominal level for both substrates and metal electrodes, i.e., the recycling level is currently assumed to be 90% for FTO/ITO and 95% for metal, since 100% recycling cannot be realistically guaranteed due to the limitation of current infrastructure. The maximum utilization efficiency for spin coating is assumed to be 90%,[29] while the nominal value is assumed to be 80%. Recycling procedures, such as selective dissolution and sonication may cause irreversible damage to the morphology of the FTO and ITO substrates, resulting in a drastic loss of performance. Despite the non-precious metal, such as Cu, being chemically stable in the selected solvents, loss of mass is still inevitable during recycling. In addition, the loss is also expected due to the metal migration during operation or other factors, indicating that the raw materials are not guaranteed to be in the original form or usable for refurbished devices. These issues reduce the effectiveness of recycling perovskite solar modules.

To quantitatively analyze these scenarios, a series of recycling levels are assigned to the investigated PSCs. The impacts of recycling levels on both primary energy consumption and global warming potential for the LBSO module are illustrated in Supplementary Figure 18. The recycling level variation (from 70% to 100%) for the substrates is greater than the metal electrode (from 90% to 100%) because the morphology completeness is relatively harder to be fulfilled. Note that the recycling of substrates is either successful or completely failed, i.e., the recycling rate for the individual substrate is either 0 or 100%. Therefore, the recycling level of substrates refers to an average proportion of successfully recycled modules. The results of the remaining perovskite PV modules are presented in the Section S12.

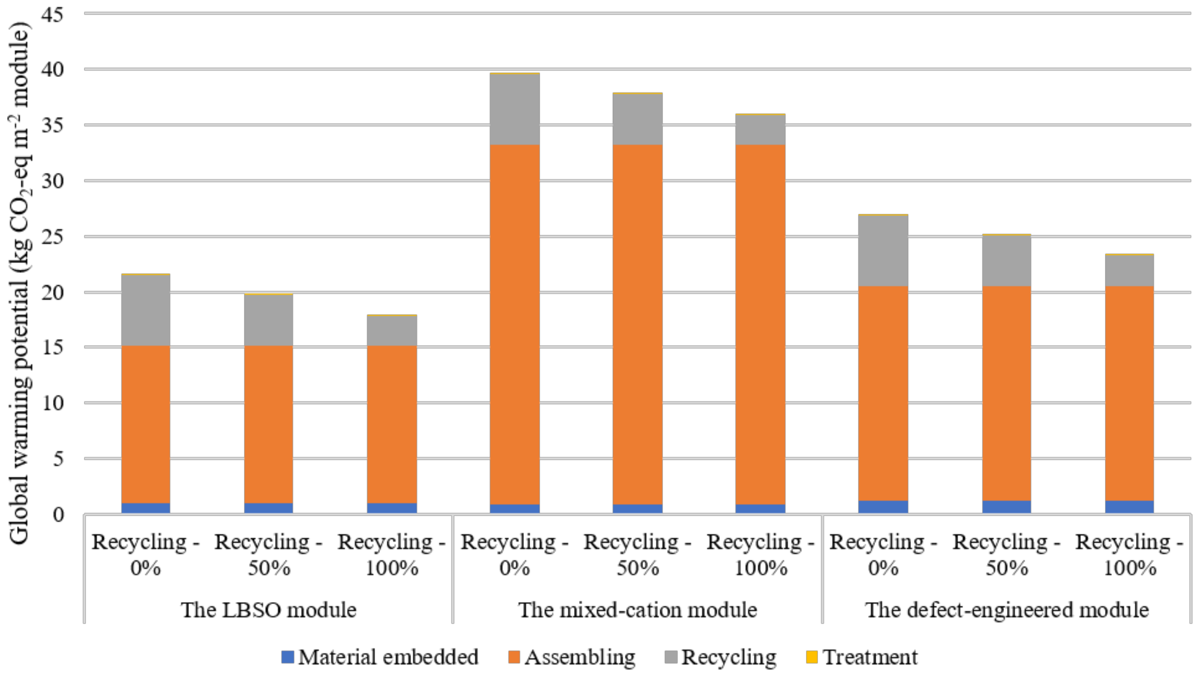


Supplementary Figure 18. Impacts of recycling levels on the primary energy consumption and global warming potential for the LBSO module (The ideal recycling scenario can be intuitively identified on the upper left corner of this heat map; the lower right corner refers to the “worst” recycling strategy).

Because the recycling strategies are derived from laboratory-scale processing steps, they are likely to encounter technical challenges in scale-up. Moreover, for recycling FTO glass via selective dissolution, some of the solvents used to remove the layers other than the electrodes and substrates can be retrieved from the solvent used to prepare the precursor solution. Earlier studies show that the direct emissions of these organic solvents have a severe photochemical oxidation effect.[1] This detrimental effect would be mitigated if organic solvents are effectively recycled and reused in the selective dissolution phase, which is quantified in terms of cumulative energy demand and global warming potential as shown in Supplementary Figure 19 and Supplementary Figure 20, respectively. Specially, we consider three scenarios with 0%, 50%, and 100% of the organic solvent recovered for the three modules that consume a large amount of organic solvent during the recycling phase. We note that the cumulative energy demand and global warming potential decrease substantially as the recycling level increases. Furthermore, because the recovered substrates could be used for new device fabrication within four to five hours,[27] the recycling infrastructure co-located with the PSC manufacturing facilities would be an appropriate blueprint for efficient manufacturing of recycled PSCs in the future.



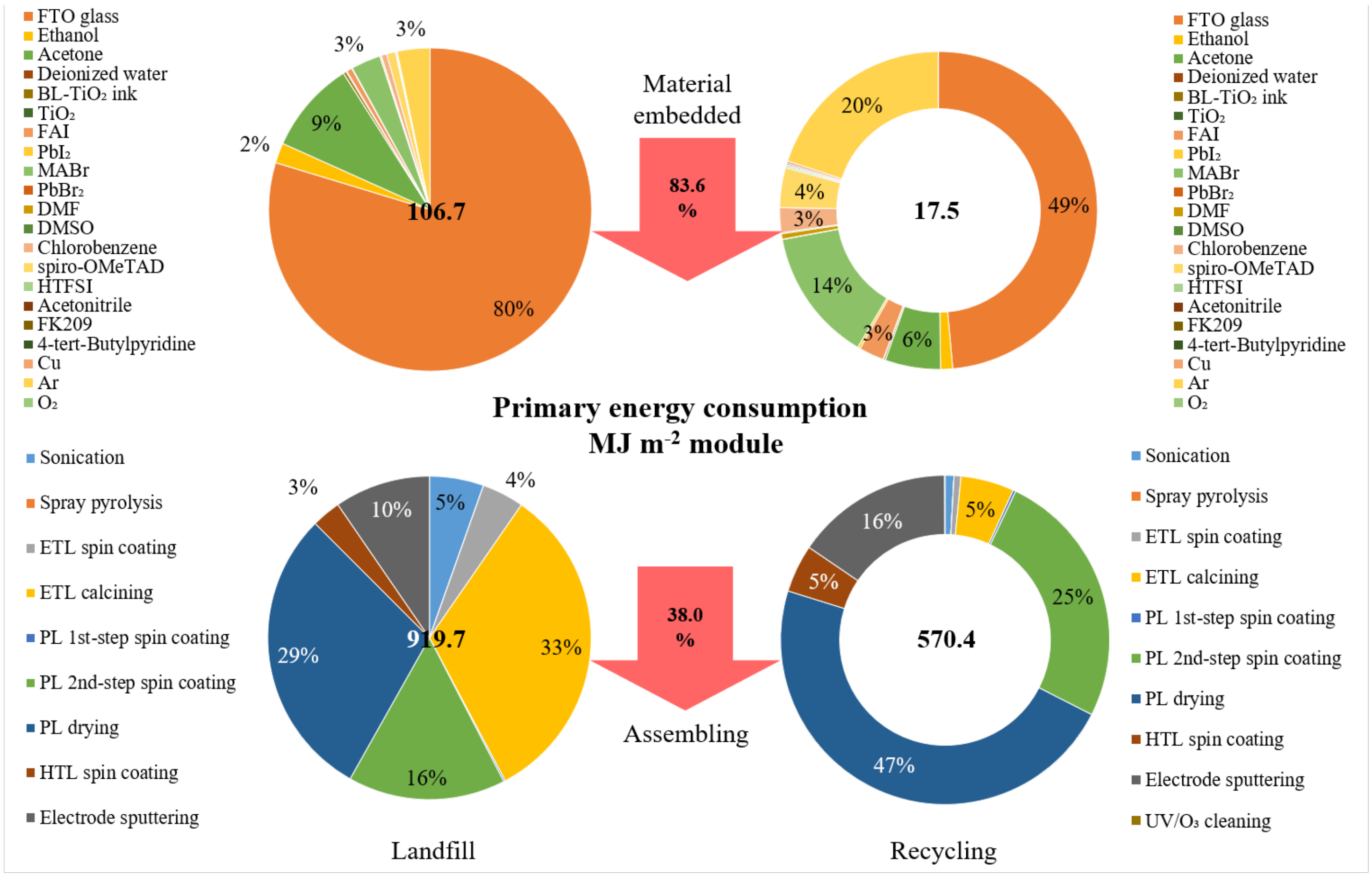
Supplementary Figure 19. Sensitivity analysis of the recycling levels of organic solvent on the cumulative energy demand for the three modules based on FTO glass.



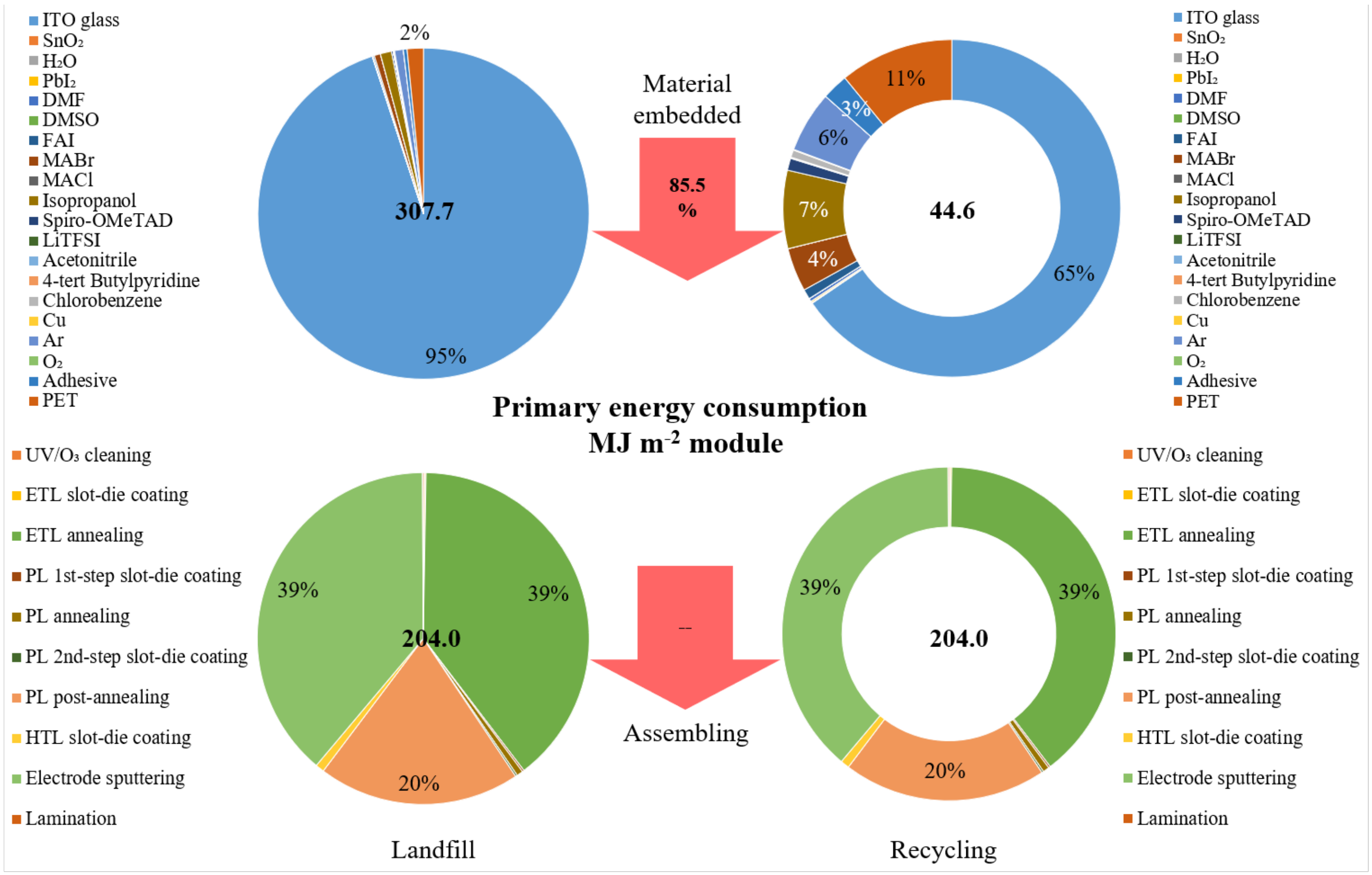
Supplementary Figure 20. Sensitivity analysis of the recycling levels of organic solvent on the global warming potential for the three modules based on FTO glass.

In spite of the relatively small environmental impacts induced by lead compounds according to the LCA results presented in this work, the use of lead is an extremely sensitive issue and may induce public concerns about the potential risks associated with lead leaking even at a relatively low concentration.[30-32] The potential negative public perception motivates the recycling of lead even though lead is not an environmental hotspot. Future work should focus on the development of efficient solvent recycling, lead recovery approaches, and robust packaging in the PSC industry, which may include incorporation of lead scavenging agents in case of failure during the lifetime and at the end-of-life phase.[33] We note incorporating such considerations in the modeling is beyond the scope of this study because there is a lack of literature addressing how the lead in such panels could be disposed of and recovered.

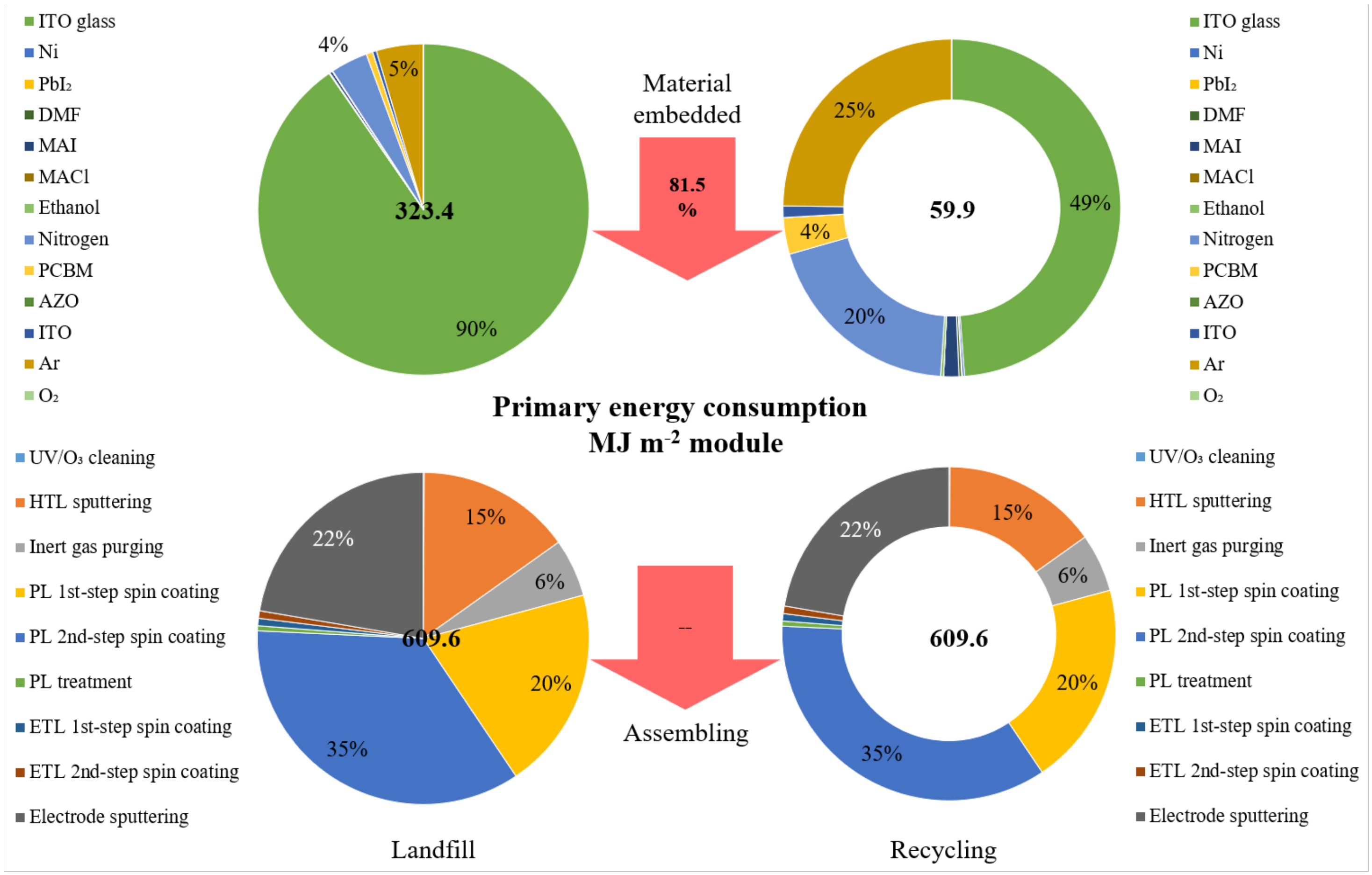
S9. Primary energy consumption comparison between landfill and recycling end-of-life scenarios



Supplementary Figure 21. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the mixed-cation module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).



Supplementary Figure 22. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the SnO_2 module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).



Supplementary Figure 23. Primary energy consumption comparison between landfill (pie charts on the left) and recycling (donut charts on the right) end-of-life scenarios for the semi-transparent module (The upper two charts refer to the primary energy consumption in material acquisition, while the lower two charts represent the energy consumption during the assembling phase of PSC preparation. The arrows in the middle reflect the variation of primary energy consumption relative to the landfill scenario).

S10. Comparison with existing PV technologies

Supplementary Table 46. Comparison between the energy payback time and lifetime for different perovskite solar cells.

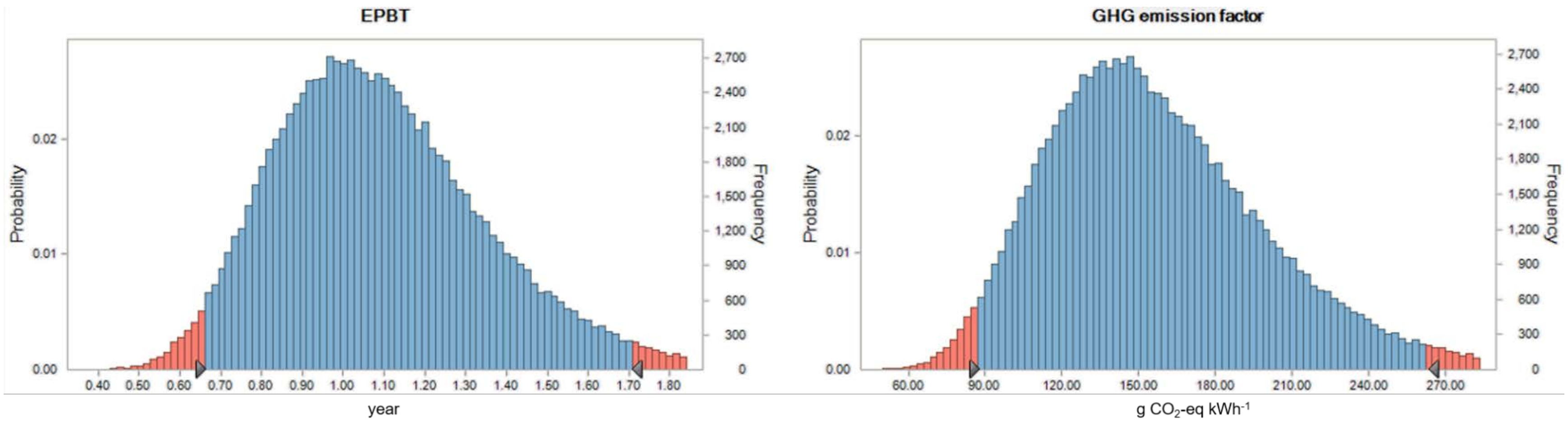
	Cumulative energy demand (MJ m^{-2})	Annual irradiation (kWh m^{-2})	Power conversion efficiency	Performance ratio	Energy payback time (year)	lifetime (year)
Espinosa et al.[34]	13,050	1,700	15.40%	0.8	1.15	15
	9,343	1,700	11.50%	0.8	1.1	15
	1,3061	1,700	15.40%	0.8	17.32	1
	9,314	1,700	11.50%	0.8	16.54	1
Gong et al.[1]	446	1,700	9.10%	0.8	0.28	2
	334	1,700	11.00%	0.8	0.18	2
Celik et al.[35]	2,550	1,700	15%	0.75	1.05	5
	3,040	1,700	15%	0.75	1.25	5

All the authors define the EPBT as the time required to generate the equivalent amount of energy that is consumed during the life cycle of PV modules. However, the system boundaries are different: Gong et al. consider a cradle-to-grave system boundary, while both Espinosa et al. and Celik et al. consider a cradle-to-gate one.[34,35] We also note that in Espinosa et al.,[34] the authors reported longer EPBT when they assumed the lifetime to be one year, which is assumed to be an error since the EPBT should be independent of the system lifetime, and the opinion is consistent with Celik et al.[35]

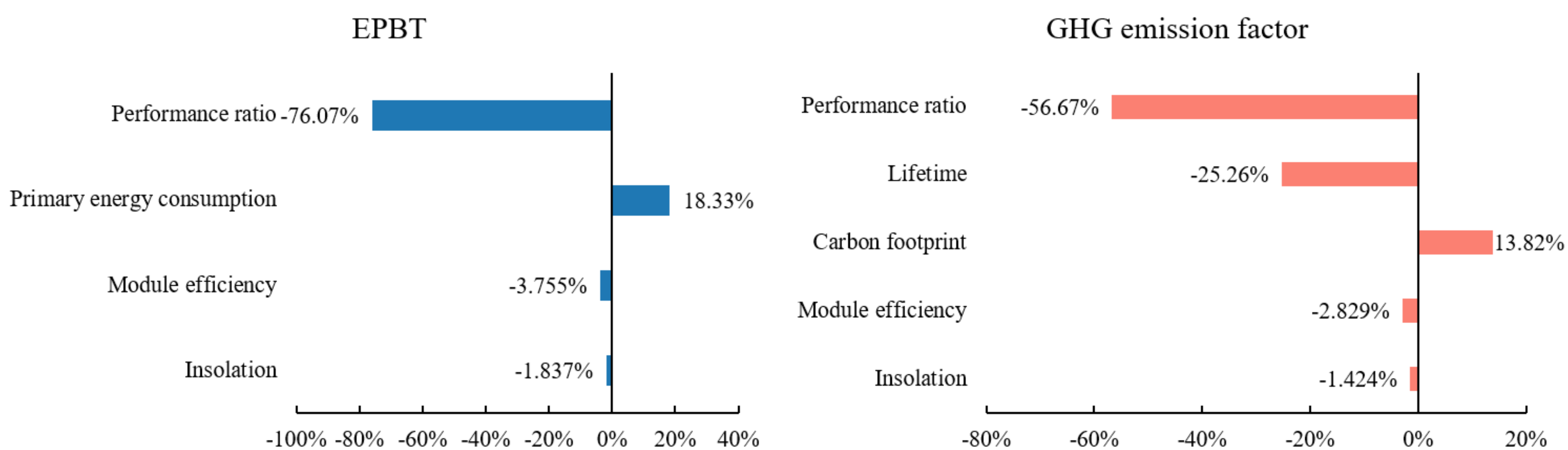
S11. Uncertainty and sensitivity analysis results

The uncertainty and sensitivity analysis results for the metal oxide module, mixed-cation module, defect-engineered module, SnO_2

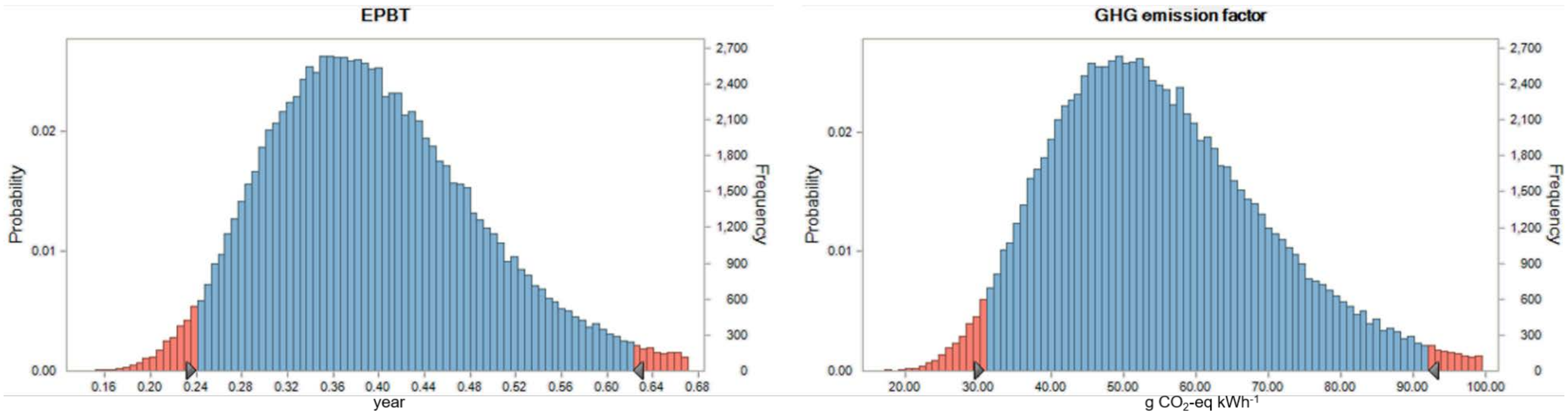
module, and semi-transparent module are shown in Supplementary Figure 24 to Supplementary Figure 33.



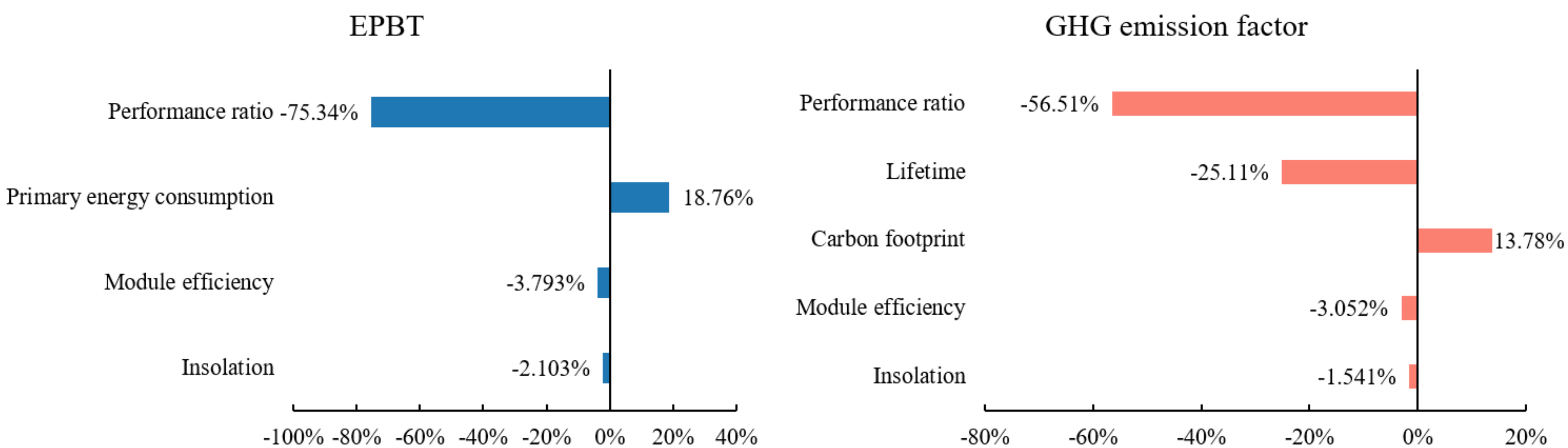
Supplementary Figure 24. Uncertainty analysis for the metal oxide module in terms of EPBT and GHG emission factor.



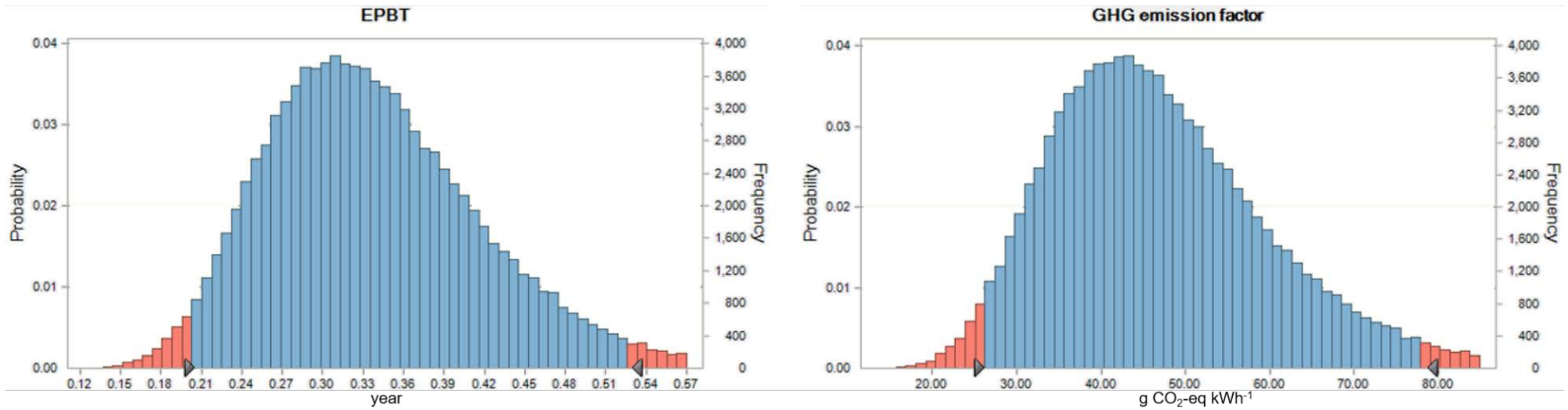
Supplementary Figure 25. Sensitivity analysis for the metal oxide module in terms of EPBT and GHG emission factor.



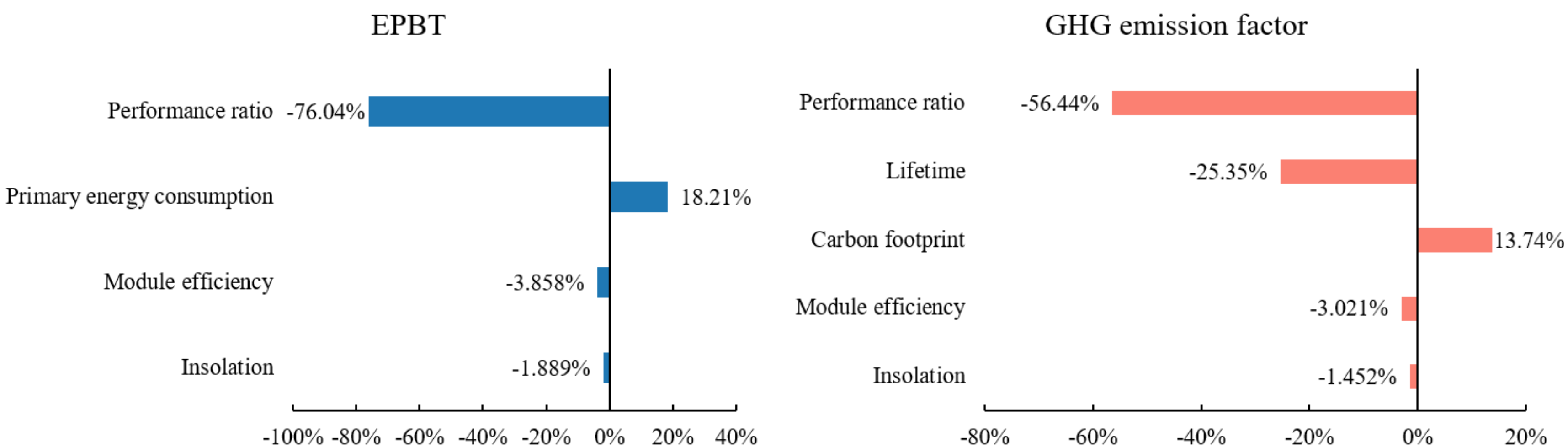
Supplementary Figure 26. Uncertainty analysis for the mixed-cation module in terms of EPBT and GHG emission factor.



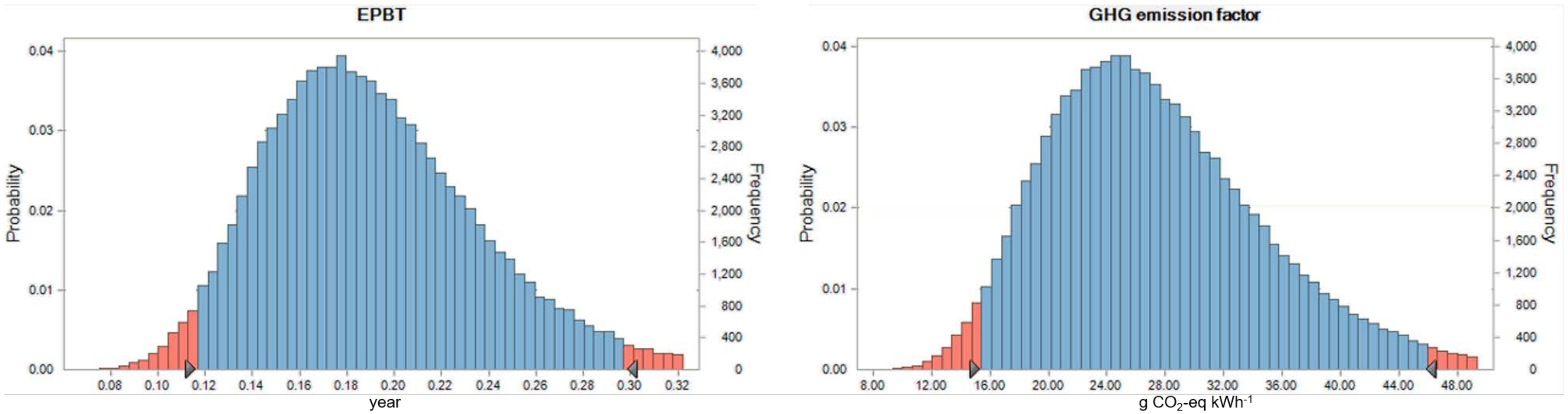
Supplementary Figure 27. Sensitivity analysis for the mixed-cation module in terms of EPBT and GHG emission factor.



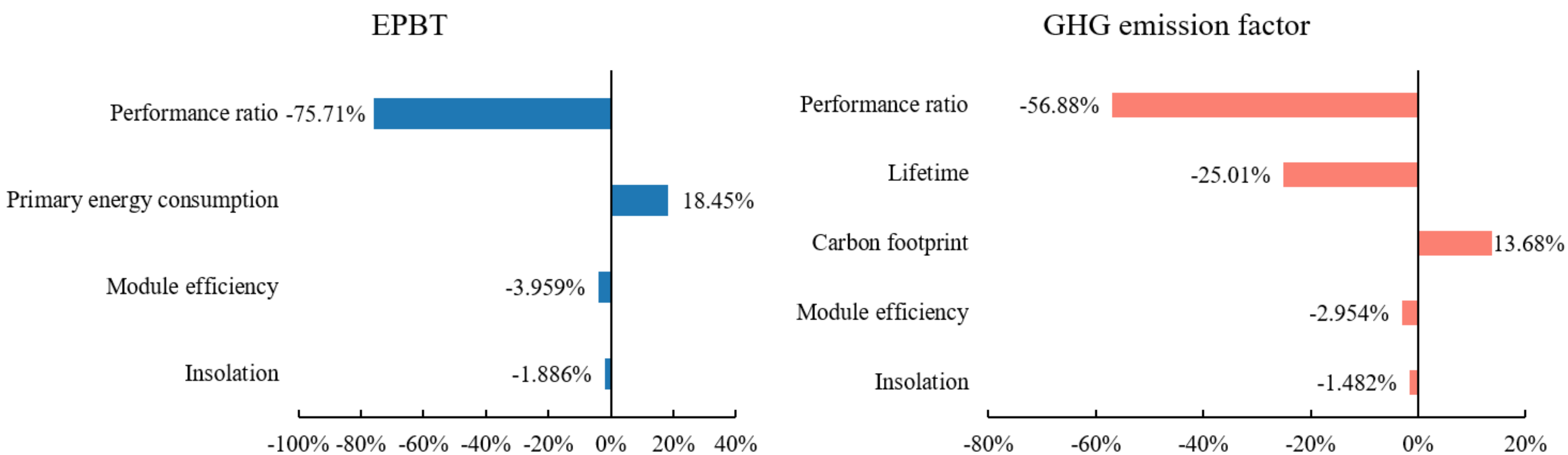
Supplementary Figure 28. Uncertainty analysis for the defect-engineered module in terms of EPBT and GHG emission factor.



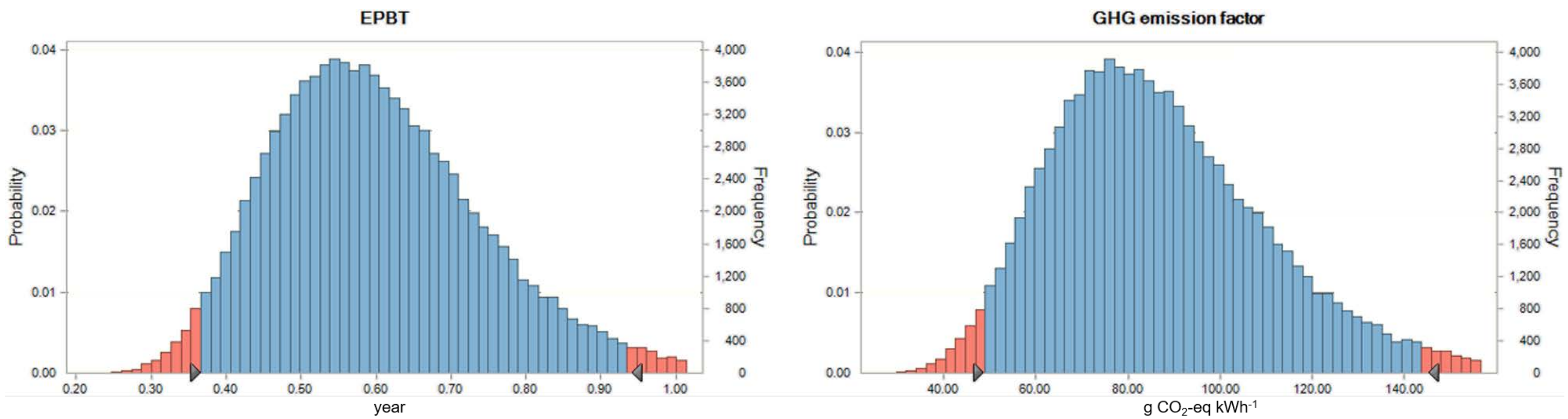
Supplementary Figure 29. Sensitivity analysis for the defect-engineered module in terms of EPBT and GHG emission factor.



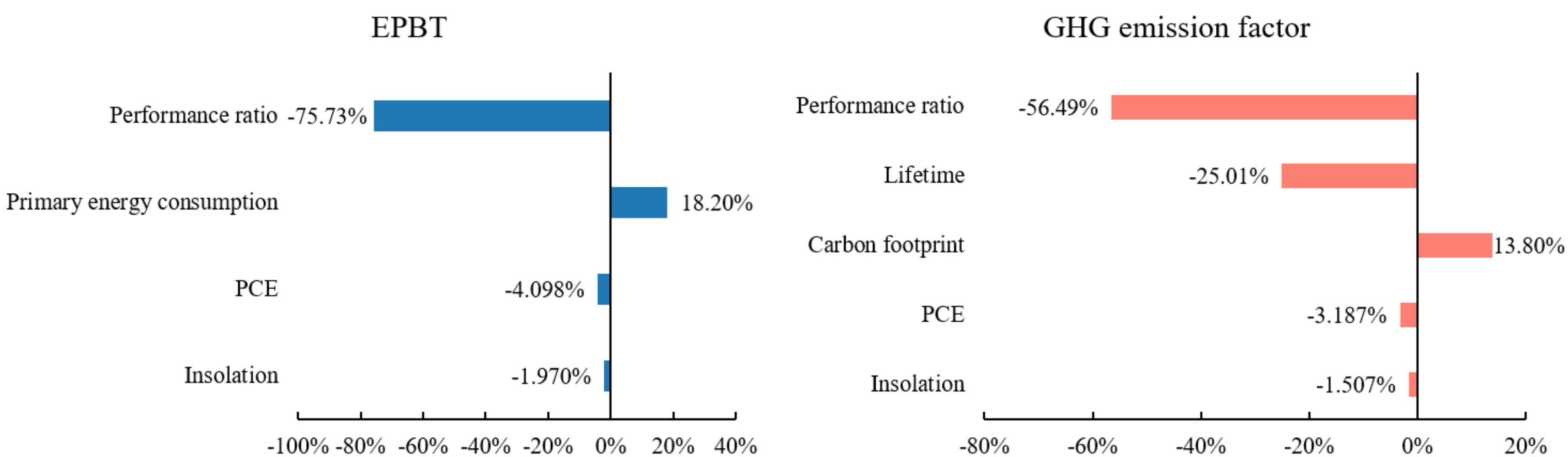
Supplementary Figure 30. Uncertainty analysis for the SnO_2 module in terms of EPBT and GHG emission factor.



Supplementary Figure 31. Sensitivity analysis for the SnO_2 module in terms of EPBT and GHG emission factor.



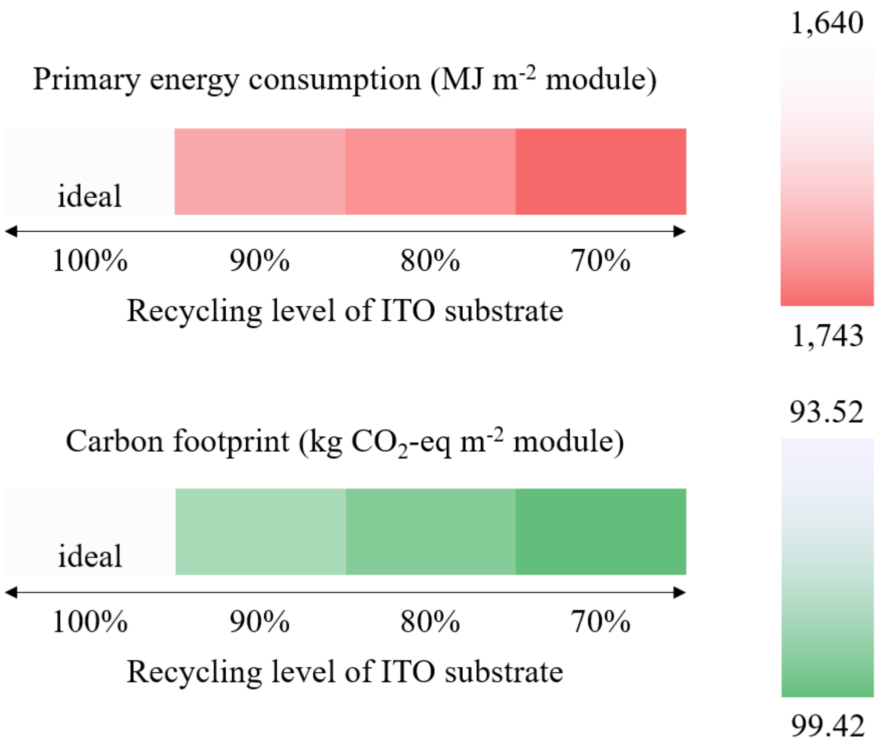
Supplementary Figure 32. Uncertainty analysis for the semi-transparent module in terms of EPBT and GHG emission factor.



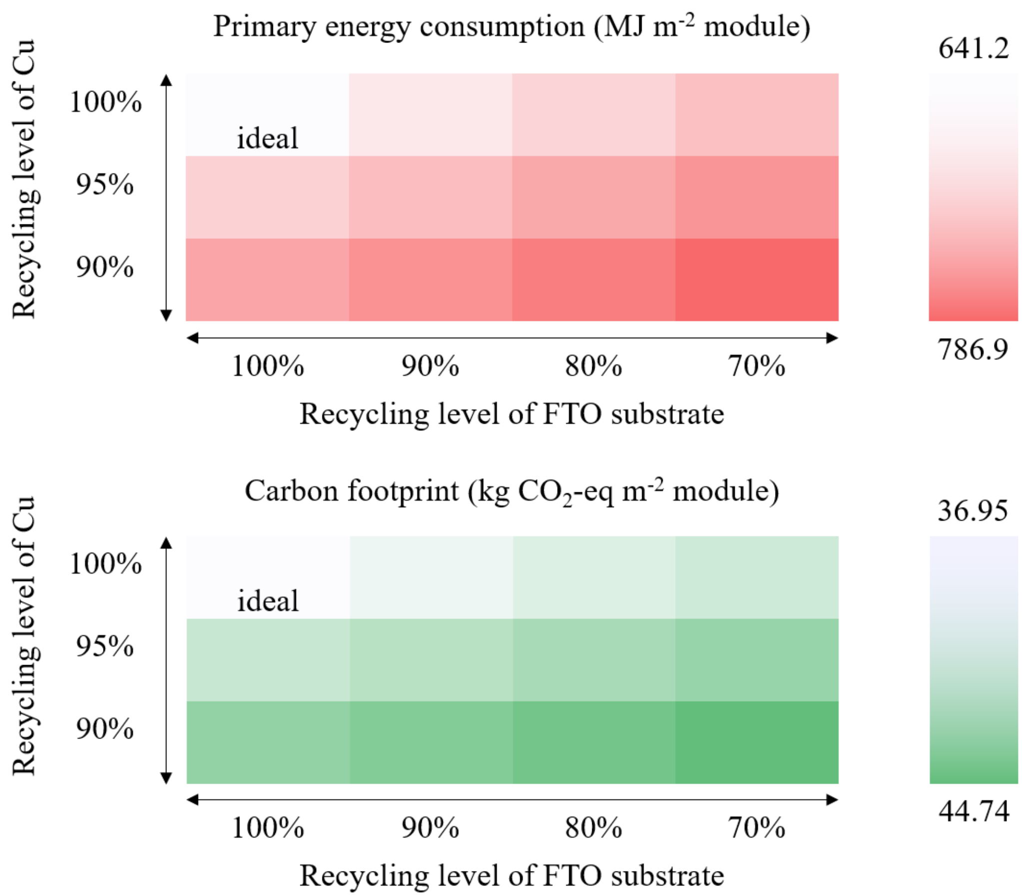
Supplementary Figure 33. Sensitivity analysis for the semi-transparent module in terms of EPBT and GHG emission factor.

S12. Impacts of recycling levels on the primary energy consumption and carbon footprint

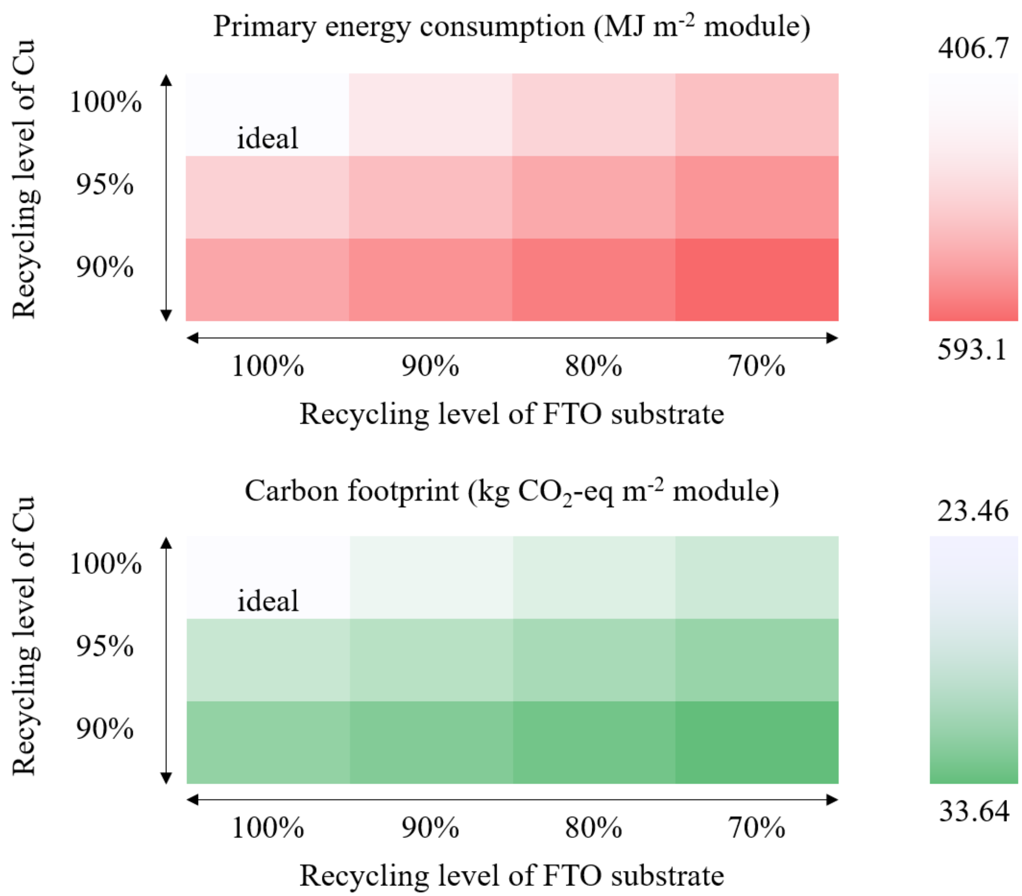
For the rest of the investigated perovskite PV modules, the impacts of recycling levels on the primary energy consumption and carbon footprint are quantified in Supplementary Figure 34 to Supplementary Figure 38, respectively. Note that for the metal oxide module, only the recycling level of ITO glass is considered, so the corresponding heat map is unidimensional.



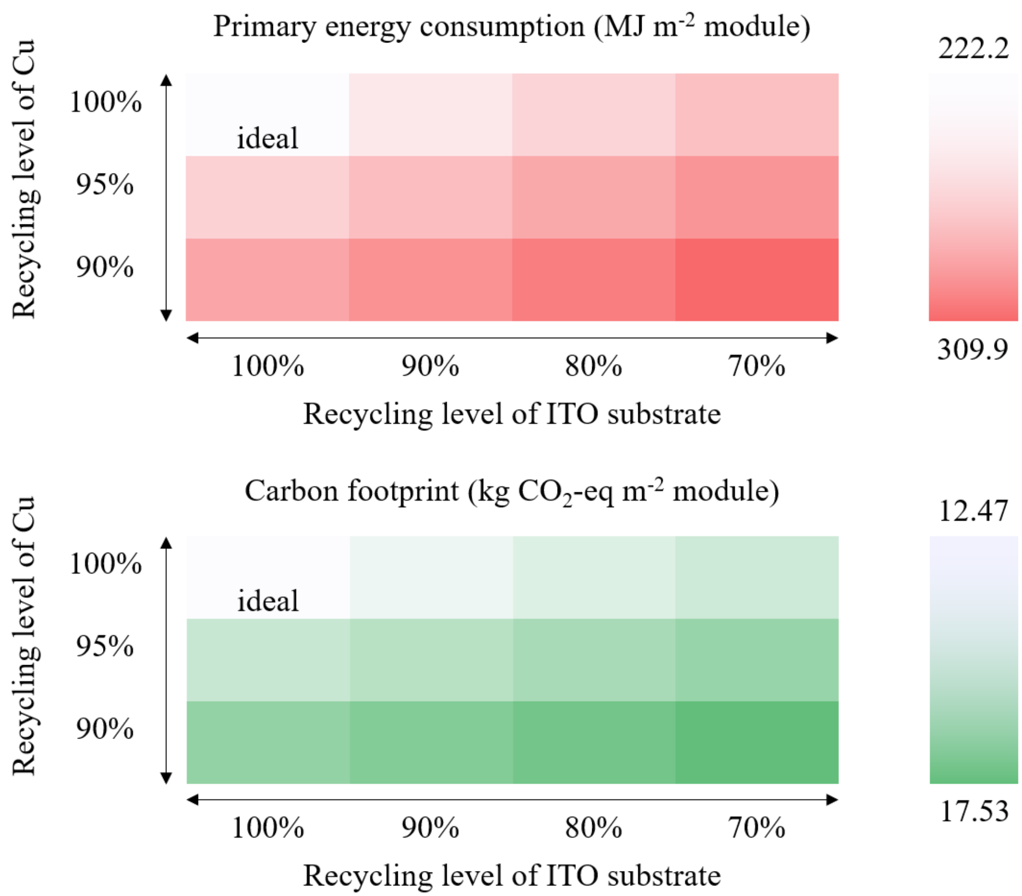
Supplementary Figure 34. Impacts of recycling levels on the primary energy consumption and carbon footprint for the metal oxide module (The ideal recycling scenario can be intuitively identified on upper left corner of this heat map; the lower right corner refers to the "worst" recycling strategy).



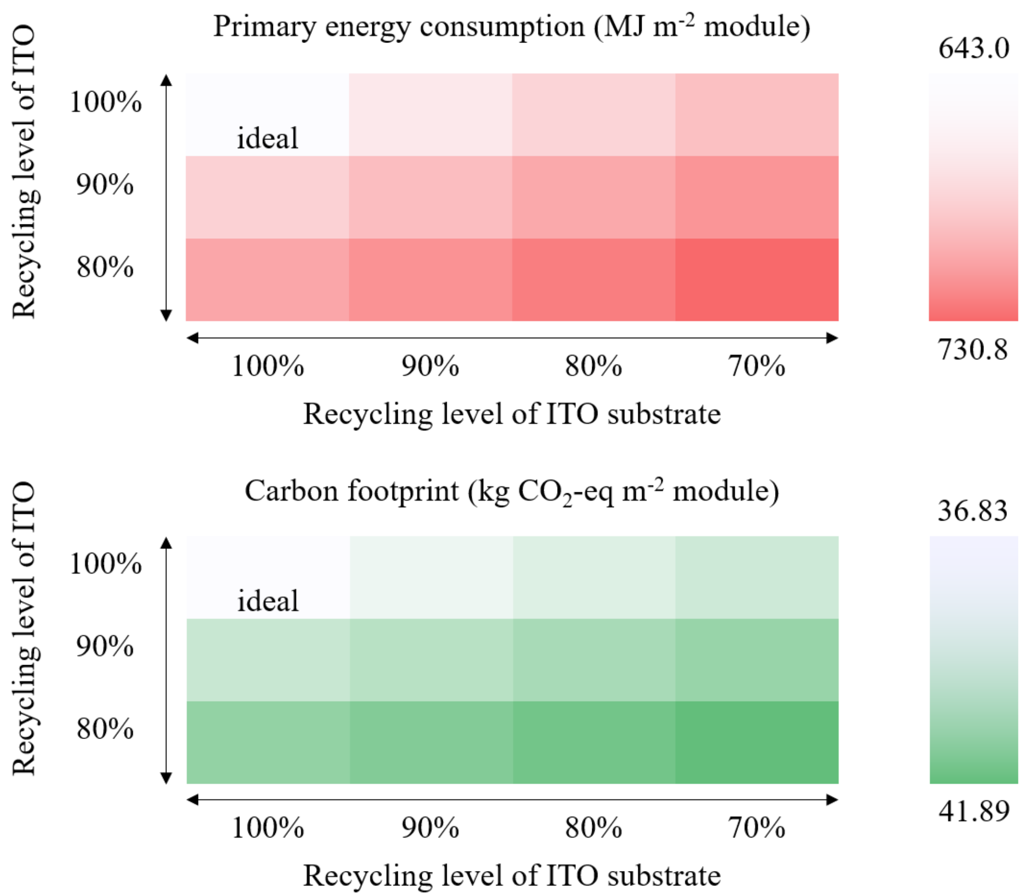
Supplementary Figure 35. Impacts of recycling levels on the primary energy consumption and carbon footprint for the mixed-cation module (The ideal recycling scenario can be intuitively identified on upper left corner of this heat map; the lower right corner refers to the “worst” recycling strategy).



Supplementary Figure 36. Impacts of recycling levels on the primary energy consumption and carbon footprint for the defect-engineered module (The ideal recycling scenario can be intuitively identified on upper left corner of this heat map; the lower right corner refers to the "worst" recycling strategy).

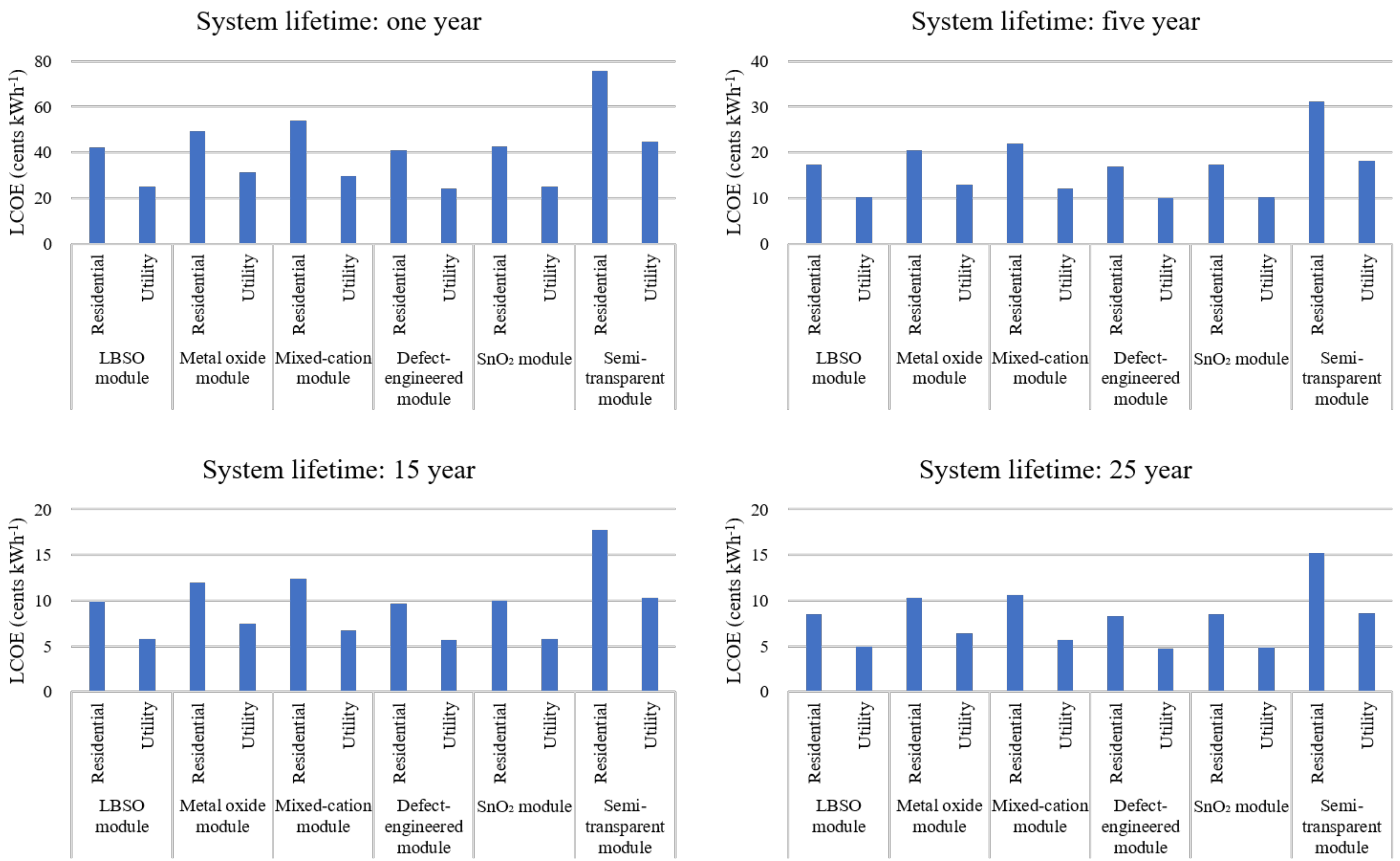


Supplementary Figure 37. Impacts of recycling levels on the primary energy consumption and carbon footprint for the SnO_2 module (The ideal recycling scenario can be intuitively identified on upper left corner of this heat map; the lower right corner refers to the "worst" recycling strategy).



Supplementary Figure 38. Impacts of recycling levels on the primary energy consumption and carbon footprint for the semi-transparent module (The ideal recycling scenario can be intuitively identified on upper left corner of this heat map; the lower right corner refers to the "worst" recycling strategy).

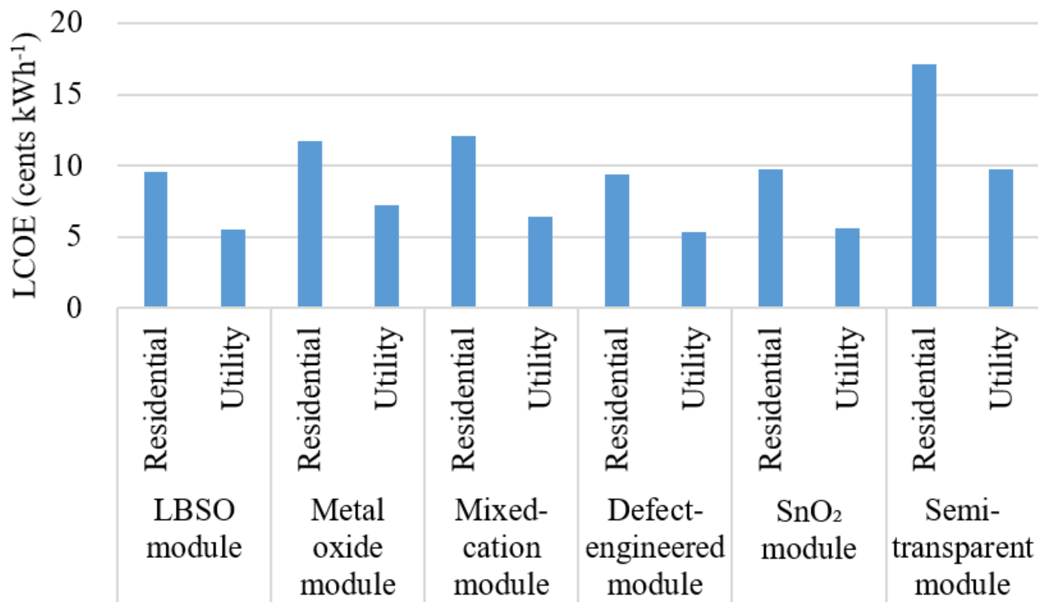
S13. Sensitivity analysis of the system lifetime on the levelized cost of electricity



Supplementary Figure 39. Sensitivity analysis of the system lifetime on the levelized cost of electricity for both residential and utility-scale systems.

S14. Levelized costs of electricity for PV systems based on recycled PV modules

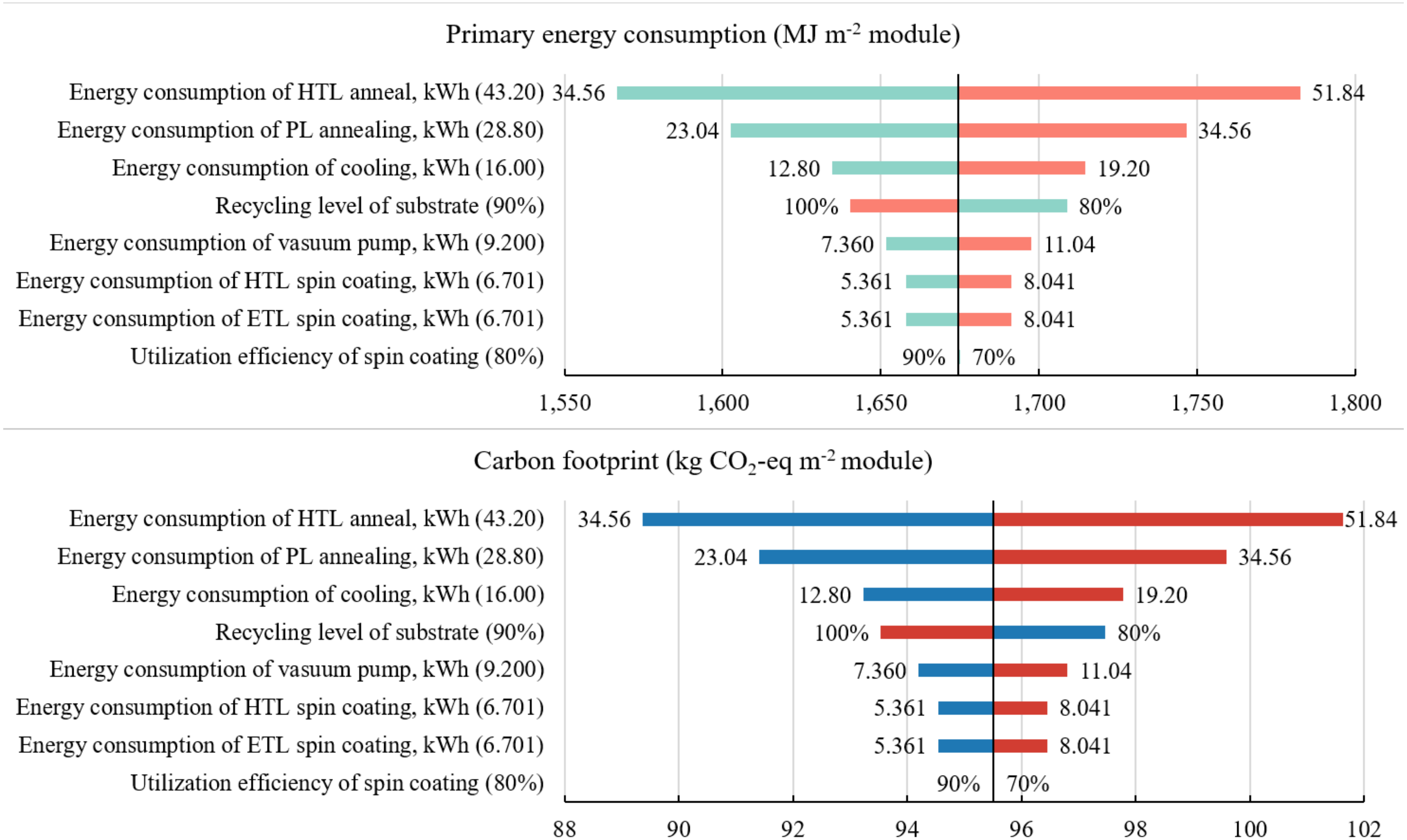
The levelized costs of electricity for PV systems based on recycled PV panels are demonstrated in Supplementary Figure 40. In the calculation, a nominal lifetime of 15 years and nominal recycling levels for key components is assumed in accordance with the main text. The levelized costs of electricity for PV systems based on recycled PV modules are 0.16 – 0.59 cents per kWh lower than the counterpart using virgin materials.



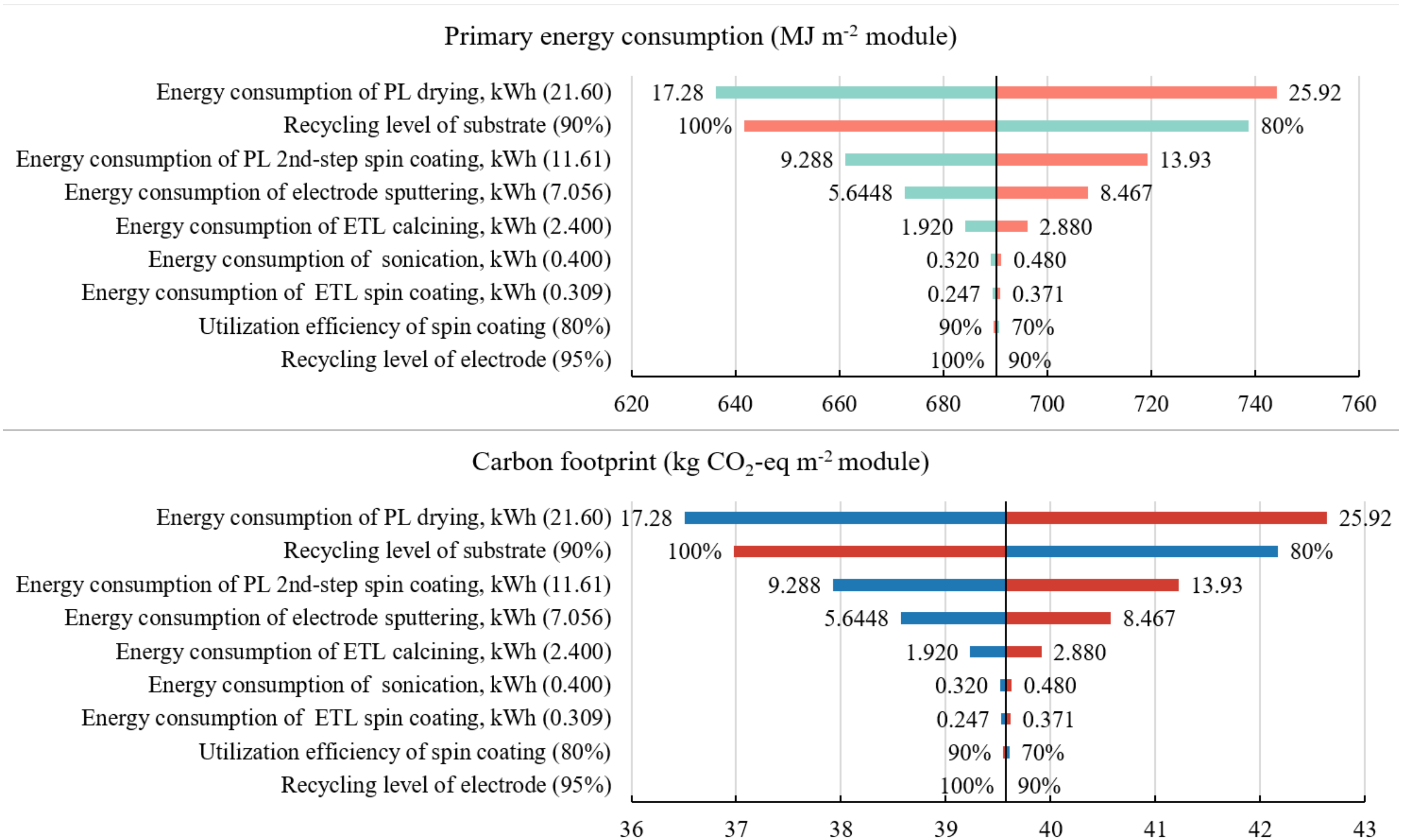
Supplementary Figure 40. Levelized cost of electricity for PV systems based on recycled PV modules.

S15. Sensitivity analysis results for recycling

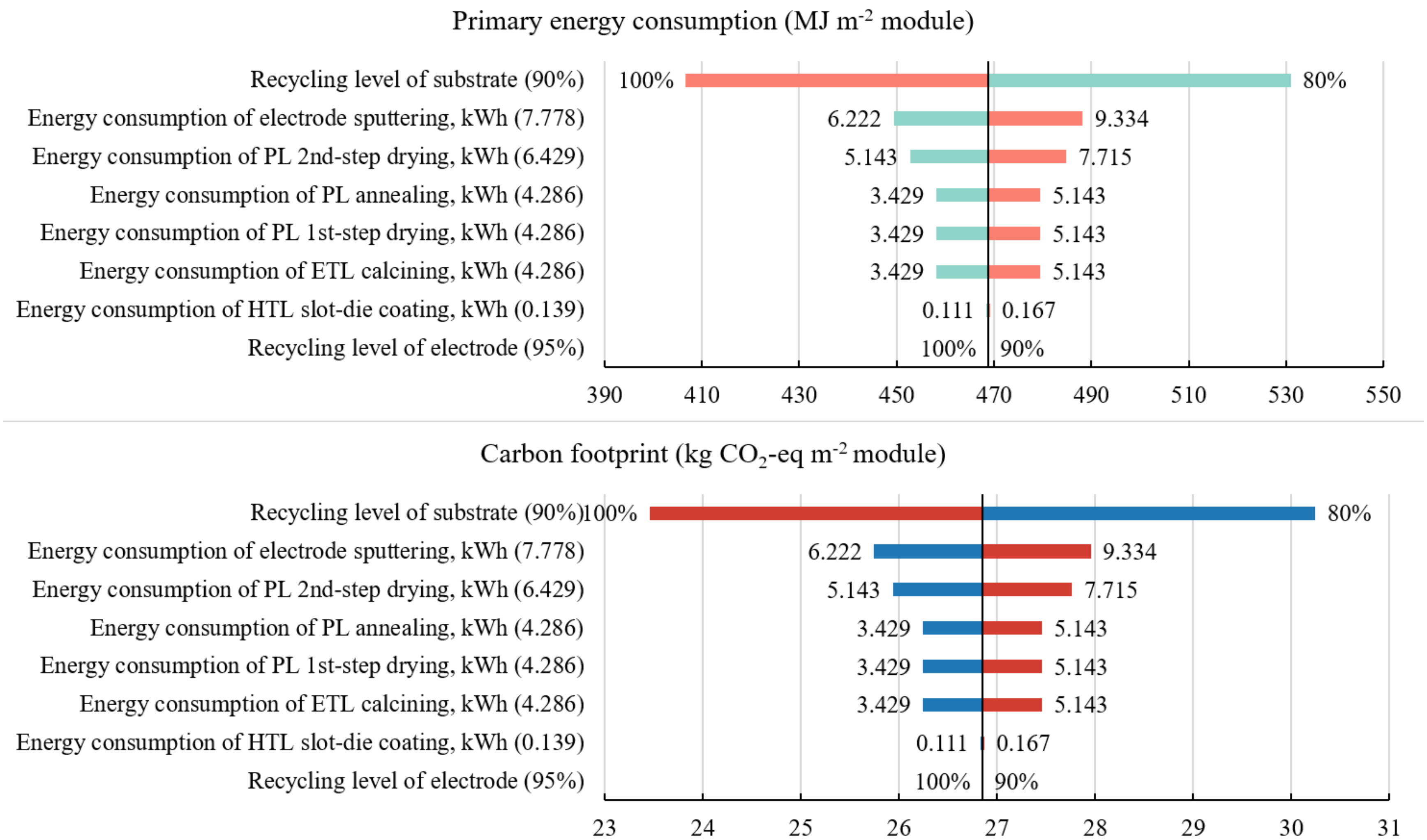
The sensitivity of recycling strategy is also quantified in terms of primary energy consumption as well as carbon footprint for the rest of the modules.



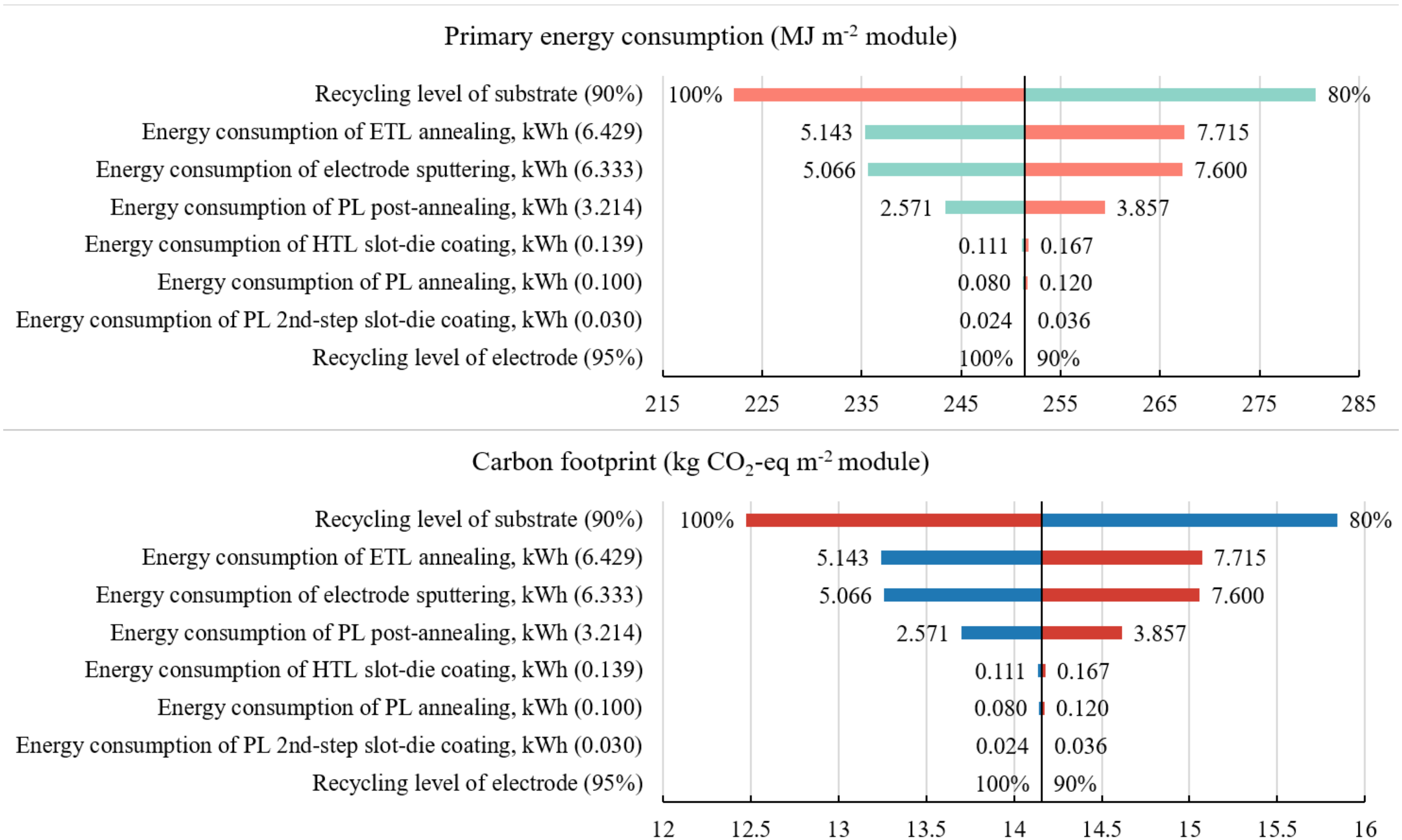
Supplementary Figure 41. Sensitivity analysis for recycling the metal oxide module in terms of primary energy consumption and carbon footprint.



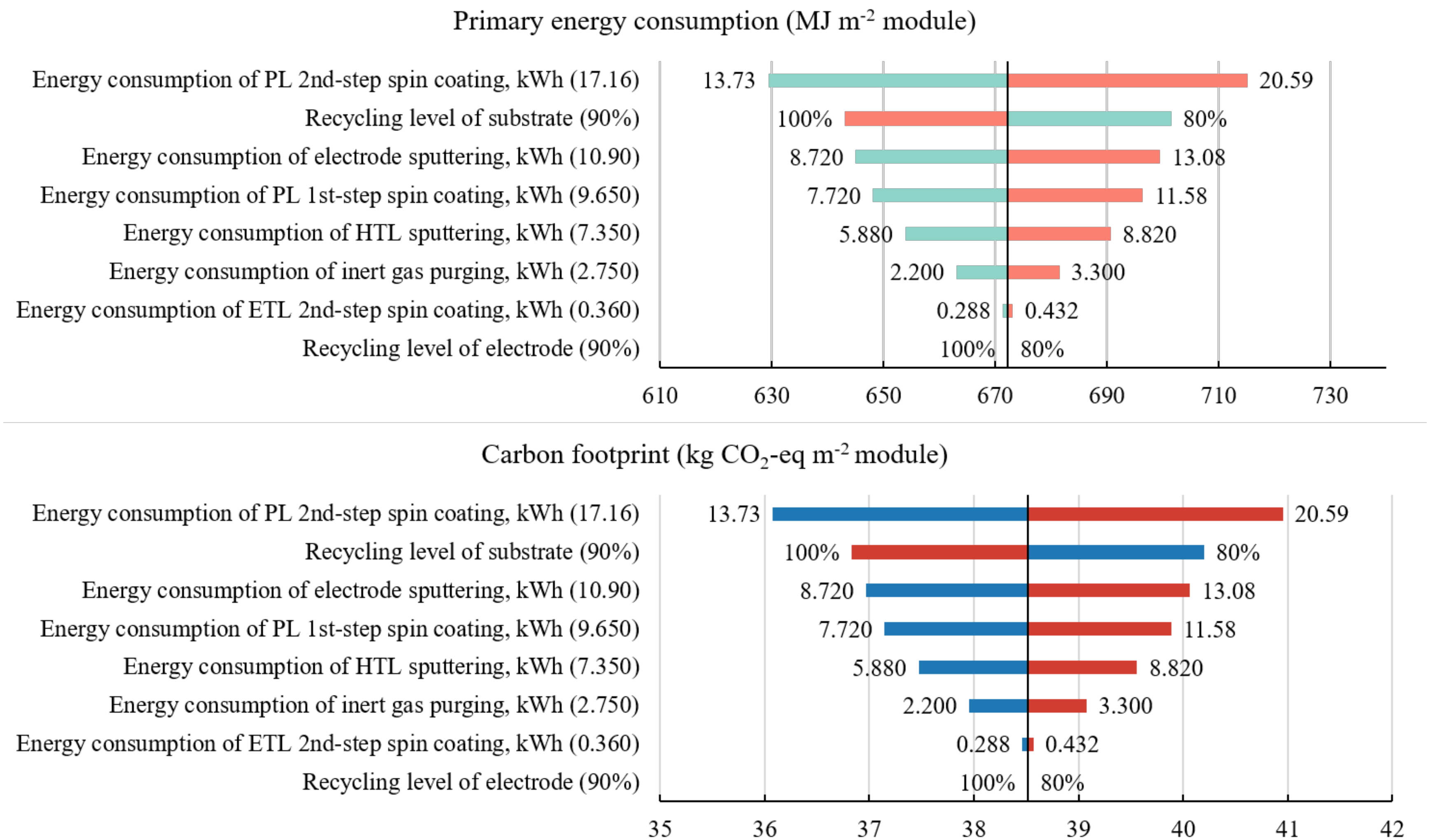
Supplementary Figure 42. Sensitivity analysis for recycling the mixed-cation module in terms of primary energy consumption and carbon footprint.



Supplementary Figure 43. Sensitivity analysis for recycling the defect-engineered module in terms of primary energy consumption and carbon footprint.



Supplementary Figure 44. Sensitivity analysis for recycling the SnO_2 module in terms of primary energy consumption and carbon footprint.



Supplementary Figure 45. Sensitivity analysis for recycling the semi-transparent module in terms of primary energy consumption and carbon footprint.

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