Supporting Information: Highly Efficient 3rd Generation Multi-Junction Solar Cells Using Silicon Heterojunction and Perovskite Tandem: Prospective Life Cycle Environmental Impacts

René Itten and Matthias Stucki

1. Life Cycle Inventory: solar cells

Tab. 1.1: Electricity demand of the different production steps in the crystalline-silicon supply chain and perovskite (or silicon heterojunction) layer deposition according to Serrano-Lujan et al. [1], Espinosa et al. [2], Gong et al. [3], Celik et al. [4], Baldassari et al. [5], Espinosa et al. [6], ecoinvent [7], IEA-PVPS [8], Louwen et al. [9], and Lunardi et al. [10]

	Electricity demand 1 m2	kWh	Cell production	PSC layer (or SHJ layer)	Wafer production	Mono-Si production	Polysilicon production	Metallurgical Si production	Total
Lab	PSC	Serrano-Lujan et al. (2015)		116'880.0					116'880.0
		Espinosa et al. (2015), VD excl back electrode		1'240.6					1'240.6
		Espinosa et al. (2015), SC excl back electrode		862.5					862.5
		Gong et al. (2015), TiO2		7.8					7.8
		Gong et al. (2015), ZnO		4.6					4.6
Lab to fab		Celik et al. (2016), HTL free, excl back electrode		108.8					108.8
		Celik et al. (2016), solution based, excl back electrode		138.7					138.7
		Celik et al. (2016), vacuum based excl back electrode		181.6					181.6
Ind		This study (Baldassari et al. 2016 / ecoinvent v3.3 2016)	14.4	17.1					35.5
Lab		OPV, Espinosa et al. (2011)	7.5						7.5
Ind	Mono-Si	Celik et al. (2016) / ecoinvent v3.3	30.2		8.5	80.3	110.5	12.5	247.0
		IEA PVPS (2015)	14.4		26.5	111.2	140.1	15.8	311.9
Ind	SHJ	Louwen et al. (2015) excl back electrode	20.2	13.9	5.7	53.6	73.6	8.3	175.2
Lab	SHJ-PSC	Lunardi et al. (2017)	14.4	876.4	26.5	111.2	140.1	15.8	1'184.3
Ind		This study (Baldassari et al. 2016 / Louwen et al. 2015)	14.4	23.7	26.5	111.2	140.1	15.8	335.6

1.1 Perovskite single junction solar cell

Tab. 1.2: Life cycle inventory of the non-bifacial single-junction organometallic halide perovskite cell (PSC) per square meter of PSC module based on Bush et al. [11], Werner et al. [12], You et al. [13], Zhu et al. [14], IEA PVPS [8], ecoinvent [7], Espinosa et al. [6], Gong et al. [3], and SimaPro [15].

	Material	Function	Application	Unit	Inputs	Utilisation rate	Reference	Name SimaPro
Single-junction perovskite solar module (framed)				**m^2**	**1**			**Photovoltaic panel, monolithic tandem SHJ-PSC, 2Terminal {RER}| PV2050 | Alloc Rec, U**
0	Substrate, cell & module							
	Glass	Substrate		kg	1.64		Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016)	Solar glass, low-iron {RER}| production | Alloc Rec, U
	Solar cell production	Front and Back Contacts	Screen printing	m^2	0.935		IEA-PVPS LCI Report (Frischknecht et al. 2015) with adjustments for wafer	photovoltaic cell, single-Si, with glass substrate instead of Si wafer, at plant/m2/RER U | PV2050
	Module production (panel)	cell inter-connection		m^2	1		IEA-PVPS LCI Report (Frischknecht et al. 2015) with adjustments for wafer	photovoltaic panel, single-Si, without wafer input via cell, at regional storage/m2/RER/I U
1	Top contact layer, Sputtering, indium tin oxide, for liquid crystal display {RER}| processing | Alloc Rec, U							Top contact layer
	Indium tin oxide	Top contact layer	Sputtering	m^3	1.12E-07	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), ITO sputtering process ecoinvent v3.3 (2016)	Sputtering, indium tin oxide, for liquid crystal display {RER}| processing | Alloc Rec, U
2	Electron transport layer, Sputtering, tin oxide SnO2, for perovskite solar cell (PSC) {RER}| processing | PV2050							Electron transport layer
	Tin oxide	Electron transport layer	Sputtering	m^3	9.35E-09	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), SnO2 sputtering based on ITO sputtering ecoinvent v3.3 (2016), own calculations for SnO2	Sputtering, tin oxide SnO2, for perovskite solar cell (PSC) {RER}| processing | PV2050
3a	Perovskite layer, Thermal evaporation, lead iodide, PbI2, physical vapour deposition, utilisation rate 20% {RER}| PV2050							Perovskite layer
	Lead-Iodide	Absorber layer	Thermal evaporation	m^3	2.34E-07	0.2	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), electricity demand and emissions based on physical vapour deposition process (ecoinvent v3.3 2016), PbI2 based on Gong et al. (2015)	Thermal evaporation, lead iodide, PbI2, physical vapour deposition, utilisation rate 20% {RER}| PV2050
3a	Perovskite layer, Slot die coating, Methyl-Ammonium-Iodied (MAI), CH3NH3I, for perovskite solar cell (PSC) {RER}| processing | PV2050							Perovskite layer
	Methl-ammonium-iodide	Absorber layer	Slot die coating	m^2	9.35E-01	0.2	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), electricity demand based on Espinosa et al. (2011), MAI based on Gong et al. (2015)	Slot die coating, Methyl-Ammonium-Iodied (MAI), CH3NH3I, for perovskite solar cell (PSC) {RER}| processing | PV2050
4	Hole transport material, Sputtering, nickel oxide NiOx, for perovskite solar cell (PSC) {RER}| processing | PV2050							Hole transport material
	Nickel oxide	Hole transport layer	Sputtering	m^3	9.35E-09	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), NiOx sputtering based on ITO sputtering ecoinvent v3.3 (2016), own calculations for NiOx	Sputtering, nickel oxide NiOx, for perovskite solar cell (PSC) {RER}| processing | PV2050

1.2 Monolithic silicon heterojunction perovskite tandem solar cell

Tab. 1.3: Life cycle inventory of the non-bifacial monolithic 2-terminal tandem cell using an organometallic halide perovskite layer and silicon heterojunction solar cell per square meter of module based on Bush et al. [11], Werner et al. [12], You et al. [13], Zhu et al. [14], IEA PVPS [8], ecoinvent [7], Espinosa et al. [6], Gong et al. [3], Louwen et al. [9], and SimaPro [15].

	Material	Function	Application	Unit	Amount	Utilisation rate	Reference	Name SimaPro
Monolithic tandem module silicon heterojunction perovskite				**m^2**	**1**			**Photovoltaic panel, monolithic tandem SHJ-PSC, 2Terminal {RER}| PV2050 | Alloc Rec, U**
0	Substrate, cell & module							
	Mono-Si wafer	Substrate		m^2	0.875			
	Solar cell production	Front and Back Contacts	Screen printing	m^2	0.93541		IEA-PVPS LCI Report (Frischknecht et al. 2015)	photovoltaic panel, single-Si, at regional storage/m2/RER/I U
	Module production	cell interconnection		m^2	1		IEA-PVPS LCI Report (Frischknecht et al. 2015)	photovoltaic panel, single-Si, at regional storage/m2/RER/I U
1	Top contact layer, indium tin oxide (ITO)							
	Indium tin oxide	Top contact layer	Sputtering	m^3	7.48E-08	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), ITO sputtering process ecoinvent v3.3 (2016)	Sputtering, indium tin oxide, for liquid crystal display {RER}| processing | Alloc Rec, U
2	Hole transport layer, nickel oxide (NiOx)							
	Nickel oxide	Hole transport material	Sputtering	m^3	9.35E-09	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), NiOx sputtering based on ITO sputtering ecoinvent v3.3 (2016), own calculations for NiOx	Sputtering, tin oxide SnO2, for perovskite solar cell (PSC) {RER}| processing | PV2050
3	Perovskite layer, Methylammonium-Lead-Iodide (MAPI), CH3NH3PbI3							
	Lead-Iodide	Absorber layer	Thermal evaporation	m^3	2.34E-07	0.2	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), electricity demand and emissions based on physical vapour deposition process (ecoinvent v3.3 2016), PbI2 based on Gong et al. (2015)	thermal evaporation, lead iodide, PbI2, 250 nm, utilisation rate 20% {RER} | PV2050
	Methyl-ammonium-iodide	Absorber layer	Slot die coating	m^2	9.35E-01	0.2	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), electricity demand based on Espinosa et al. (2011), MAI based on Gong et al. (2015)	Slot die coating, Methyl-Ammonium-Iodied (MAI), CH3NH3I, for perovskite solar cell (PSC) {RER}| processing | PV2050
4	Electron transport layer Tin oxide (SnO2)							
	Tin oxide	Electron transport layer	Sputtering	m^3	9.35E-09	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), SnO2 sputtering based on ITO sputtering ecoinvent v3.3 (2016), own calculations for SnO2	Sputtering, tin oxide SnO2, for perovskite solar cell (PSC) {RER}| processing | PV2050
5	Emitter and Passivation a-Si							
	a-Si	Texturing and cleaning		m^2	9.35E-01		Louwen et al. (2015)	texturing and cleaning, photovoltaic cell, silicon heterojunction SHJ {RER} | PV2050 | Alloc Rec, U
	a-Si	Thinfilm depositon a-Si	PECVD	m^2	9.35E-01		Louwen et al. (2015)	Thinfilm deposition, a-SI, Plasma enhanced vapour deposition, PECVD, photovoltaic cell, silicon heterojunction SHJ {RER} | PV2050 | Alloc Rec, U
	a-Si	Curing		m^2	9.35E-01		Louwen et al. (2015)	curing, photovoltaic cell, silicon heterojunction SHJ {RER} | PV2050 | Alloc Rec, U
	a-Si	Gas abatement		m^2	9.35E-01		Louwen et al. (2015)	gas abatement, photovoltaic cell, silicon heterojunction SHJ {RER} | PV2050 | Alloc Rec, U
6	Back contract layer indium tin oxide (ITO)							
	Indium tin oxide	Back contact layer	Sputtering	m^3	9.35E-08	0.15	Bush et al. (2017), Werner et al. (2016), You et al. (2016), Zhu et al. (2016), ITO sputtering process ecoinvent v3.3 (2016)	Sputtering, indium tin oxide, for liquid crystal display {RER}| processing | Alloc Rec, U

2. Life Cycle Inventory: deposition process

2.1 Nickel oxide

Tab. 2.1: Life cycle inventory of the nickel oxide production based on ecoinvent v3.3 [7], SimaPro [15], and our own calculations.

Name SimaPro	Unit	Amount	Comment and references
Nickel oxide, NiO {GLO}	**kg**	**1**	
Resources			
Oxygen in air	kg	0.225	based on stochiometric principles. Process efficiency assumed 95%.
Water, cooling, unspecified natural origin, GLO	m^3	2.40E-02	Estimation.
Material			
Chemical factory, organics {GLO}| market for | Alloc Rec, U	p	8.00E-10	Estimation.
Nickel, 99.5% {GLO}| market for | Alloc Rec, U	kg	8.28E-01	based on stochiometric principles. Process efficiency assumed 95%.
Isopropanol {GLO}| market for | Alloc Rec, U	kg	2.07E-03	
Energy			
Heat, in chemical industry {RER}| market for | Alloc Rec, U	MJ	5.28E-01	Estimation.
Heat, in chemical industry {RoW}| market for | Alloc Rec, U	MJ	2.67E+00	
Emissions to air			
Water/m3	m^3	9.30E-03	
Emissions to water			
Water, GLO	m^3	1.47E-02	

2. 2 Sputtering tin dioxide

Tab. 2.2: Life cycle inventory of tin oxide sputtering process based on Classen et al. [16], Hischier et al. [17], ecoinvent v3.3 [7], SimaPro [15], and our own calculations.

Name SimaPro	Unit	Amount	Comment and references
Sputtering, tin oxide SnO2, for perovskite solar cell (PSC) {RER}	**m^3**	**1**	
Material			
Building, multi-storey {GLO}| market for | Alloc Rec, U	m^3	1.47E+02	
Tin dioxide {GLO}| market for | Alloc Rec, U	kg	4.54E+04	sputteting target utilisation rate 15% as in sputtering ITO, Dichte Sno2 6850 kg / m3
Chemical factory {GLO}| market for | Alloc Rec, U	kg	5.88E+02	
Energy			
Electricity, medium voltage {ENTSO-E}| market group for | Alloc Rec, U	kWh	2.93E+07	same electricity demand as ITO sputtering

2.3 Sputtering nickel oxide

Tab. 2.3: Life cycle inventory of nickel oxide sputtering process based on Classen et al. [16], Hischier et al. [17], ecoinvent v3.3 [7], SimaPro [15], and our own calculations.

Name SimaPro	Unit	Amount	Comment and references
Sputtering, nickel oxide NiOx, for perovskite solar cell (PSC)	**m^3**	**1**	
Material			
Building, multi-storey {GLO}| market for | Alloc Rec, U	m^3	1.47E+02	
Nickel oxide, NiO {GLO}	kg	4.45E+04	sputteting target utilisation rate 15% as in sputtering ITO, density NiO 6670 kg/m3
Chemical factory {GLO}| market for | Alloc Rec, U	kg	5.88E+02	
Energy			
Electricity, medium voltage {ENTSO-E}| market group for | Alloc Rec, U	kWh	2.93E+07	same electricity demand as ITO sputtering

2.4 Thermal evaporation lead iodide

Tab. 2.4: Life cycle inventory for the thermal evaporation of lead iodide based on Classen et al. [16], Hischier et al. [17], ecoinvent v3.3 [7], SimaPro [15], and our own calculations.

Name SimaPro	Unit	Amount	Comment and references
Thermal evaporation, lead iodide, PbI2, physical vapour deposition {RER}| PV2050	**m^3**	**1**	
Resources			
Water, unspecified natural origin, RER	m^3	2.25E+05	
Material			
Metal coating facility {GLO}| market for | Alloc Rec, U	p	4.10E-03	
Oxygen, liquid {RER}| market for | Alloc Rec, U	kg	1.12E+04	Assumption
Lead-II-iodide, PbI2, perovskit layer, PSC {RER}	kg	1.23E+04	Utilisation ration 50%, density PbI2 6160 kg/m3
Nitrogen, liquid {RER}| market for | Alloc Rec, U	kg	2.24E+04	
Energy			
Electricity, medium voltage {ENTSO-E}| market group for | Alloc Rec, U	kWh	1.48E+07	
Emissions to air			
Water/m3	m^3	1.34E+04	
Emissions to water			
Water, RER	m^3	7.58E+04	

2.5 Slot die coating methyl ammonium iodide

Tab. 2.5: Life cycle inventory for the slot die coating of methyl ammonium iodide based on ecoinvent v3.3 [7], SimaPro [15], Espinosa et al. [6], and our own calculations.

Name SimaPro	Unit	Amount	Comment and references
Slot die coating, Methyl-Ammonium-Iodied (MAI), CH3NH3I, for perovskite solar cell (PSC) {RER}	m^2	**1**	
Material			
methylammonium-iodide, MAI, CH3NH3I, perovskit layer, PSC{RER}	kg	6.60E-04	stoichiometric calculation, 0.000528 kg MAI in CH3NH3PI3; Density 4119 kg/m3, layer thickness 500 nm, utilisation rate 80%, Density MAI: 1100 kg/m3
Photovoltaic panel factory {GLO}| market for | Alloc Rec, U	p	4.00E-06	Assumption
Nitrogen, liquid {RER}| market for | Alloc Rec, U	kg	1.57E+01	Assumption
Isopropanol {GLO}| market for | Alloc Rec, U	kg	1.03E-02	6wt-% solution MAI in isopropanol / 2 propanol
Energy			
electricity, medium voltage, production ENTSO, at grid/ENTSO U	kWh	2.64E+00	Espinsoa et al. (2011) preparation 1.48 Wh, slot die 455.37Wh, Drying 2185 Wh
Emissions to air			
Heat, waste	MJ	9.50E+00	calculated
2-Propanol	kg	4.14E-02	calculated

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