Supplementary Information

Table S1. Process Sequence for different scenarios.

	A: CIGS Glass	B: CZTS Glass	C: CZTS stainless steel	D: CZTS PI	Cost data source
Upload&Wash Backglass	✔	✔			[1]
Prepare Stainless Steel			✔		Manufacturer Communication
Prepare PI				✔	Supplier Communication
Sputter Ti barrier			✔		[2]
Sputter Mo	✔	✔	✔	✔	[1]
Sputter NaF			✔	✔	[3]
P1 scribe (mechanical)	✔	✔	✔	✔	[1]
Sputter CIGS	✔				[1]
Sputter CZTS		✔	✔	✔	[4]
Selenization (Rapid Thermal Processing)	✔				[1]
Sulfurization		✔	✔		[5]
Sulfurization (low T)				✔	[5]
CdS buffer (chemical bath deposition)	✔	✔	✔	✔	[1]
P2 scribe (mechanical)	✔	✔	✔	✔	[1]
Sputter TCO	✔	✔	✔	✔	[1]
P3 scribe (mechanical)	✔	✔	✔	✔	[1]
Edge delete (mechanical)	✔	✔	✔	✔	[1]
Solder Busbar & Tape	✔	✔	✔	✔	[1]
ETFE			✔	✔	[6]
PET			✔	✔	[7]

TPO			✔	✔	[8]
Upload &Wash Front glass	✔	✔			[1]
Stack EVA and glass	✔	✔			[1]
Lamination	✔	✔	✔	✔	[1]
Trim	✔	✔	✔	✔	[1]
Frame	✔	✔			[1]
J-Box and label	✔	✔	✔	✔	[1]
LS & Hi-pot test	✔	✔	✔	✔	[1]

Table S2. Cost breakdown of absorber layers for CIGS (first four rows) and CZTS.

	Ratio	Thickness	Material cost per kg	Cost per m^2
Cu	1	1.5μm	6.83	0.10
In	0.7	1.5μm	131.58	1.37
Ga	0.3	1.5μm	138.69	0.62
Se	2	1.5μm	14.22	0.42
Cu	2	0.75μm	6.83	0.10
Zn	1	0.75μm	2.59	0.02
Sn	1	0.75μm	20.06	0.15
S	4	0.75μm	0.4	0.01

Table S3. Input data used for the cost model

	Material cost range ($/$m^2$)	Non-material cost range ($/$m^2$)
Substrate Glass	3.41 (2.73 – 4.10)	0.88 (0.70 – 1.06)
Mo layer	1.04(0.83-1.25)	1.95(1.56-2.34)
P1 laser Scribe	0.00	0.69(0.55-0.83)
CuGaIn layer	2.51(2.01-3.01)	2.05(1.64-2.46)
Selenization	4.21(3.37-5.06)	9.33(7.47-11.20)
CdS buffer	0.32(0.26-0.38)	1.44(1.15-1.73)
P2 Mechanical Scribe	0.00	0.69(0.55-0.83)
TCO layer	1.49(1.19-1.79)	2.32(1.86-2.78)
P3 Mechanical Scribe	0.00	0.69(0.55-0.83)
Edge Delete	0.00	1.33(1.07-1.60)
Busbars and Tape	1.23(0.98-1.47)	0.99(0.79-1.18)
Front Glass	8.21(6.57-9.86)	0.43(0.34-0.51)
Stack EVA and back glass	3.44(2.75-4.13)	0.48(0.38-0.58)
Laminate Front and Back Glass	0.00	2.16(1.73-2.59)

Trim	0.00	0.48(0.38-0.58)
Frame	5.71(4.57-6.85)	0.75(0.60-0.90)
Attach J-Box & sticker Lable	0.00	1.33(1.07-1.60)
Light Soaking & Hi-Pot Test	0.24(0.19-0.29)	0.32(0.26-0.38)
NaF layer	0.00(0.00-0.00)	0.08(0.06-0.10)
Ti layer	0.10(0.08-0.12)	0.40(0.32-0.48)
CuZnSn layer	0.27(0.22-0.32)	1.40(1.20-1.60)
Sulfurization	0.12(0.10-0.14)	6.53(5.60-7.46)
Substrate SS	3.98(3.62-4.34)	0.88(0.70-1.06)
Substrate PI	14.11(11.29-16.94)	0.88(0.70-1.06)
Sulfurization (low T)	0.12(0.10-0.14)	6.53(4.57-10.45)
ETFE layer	3.44(2.75-4.13)	0.38(0.26-0.49)
PET layer	1.07(0.86-1.28)	0.12(0.08-0.15)
TPO layer	3.80(1.80-6.51)	0.42(0.29-0.54)

Cost estimates:

- **Substrate**

For processes A and B, the glass substrate is assumed to account for the same cost as the reference paper[1]. For process C, Ferrite stainless steel 430 supplied for the PV industry as substrates from Baosteel is \$3.6-4.3/m^2. UPILEX s-25 from UBE INDUSTRIES, LTD. is a commercial product with high-temperature resistance, good chemical stability, and smooth surface, which is assumed to be utilized in process D as the substrate. The price ranging from different quotations is \$11.3-16.9/m^2.

For the preparation costs of each substrate, we know the cost of glass (which includes glass washing) is \$0.88/m^2[9]. Due to the limited fluctuations in the cost of cleaning and cutting different substrates, it is assumed here that the preparation costs of stainless steel and plastic substrates are the same, and with a higher uncertainty of ±30%.

- **Barrier and sodium-source layers**

For the material cost of NaF and Ti, it is not reliable to directly calculate the sputtering target cost due to different target utilization. Here we assumed the cost of the Mo layer is related to the material cost of Mo powder and its thickness. Then after obtaining the price of sodium fluoride and titanium powder and the thickness of the coating, the cost of the NaF and Ti layers can be calculated by the same ratio. The reason for choosing powder for cost calculation is that the price of powder is mostly determined by elements, which reduces errors caused by selecting different suppliers. The price of powder with the same purity of different metals is used for comparison. The sources of Ti and NaF are \$10-70/kg and \$500-1000/ton from suppliers, respectively. The material cost of Ti and NaF calculated as \$ 0.1/m^2 and \$ 0.0004/m^2, respectively, based on the differences in thickness and price of Mo layer and required layer.

The equipment running cost will be related primarily to its thickness. It is assumed that the barrier layer, the sodium-containing layer, and the absorption layer have a similar deposition rate in the industrial production line. Since the non-material cost for sputtering 250nm Mo is \$2/m^2, depositing 50nm Ti and 10nm NaF layer cost \$0.4/m^2 and \$0.08/m^2, respectively.

- **Absorber**

For the sputtering of the CZTS absorber layer, the material cost can be derived from CIGS. The stoichiometric ratio of CZTS is close to 2: 1: 1: 4 and 1: 0.7: 0.3:2 for CIGS. The price of the CZTS absorption layer can be obtained by weighting the metal cost according to its proportion. The resulting price is divided by two since the required thickness is 0.7-0.8μm instead of 1.5μm in the literature. Prices for all metals were quoted from different periods and statistically averaged. The resulting costs are summarized in Table S2.

As for non-material costs, first of all, compared with CIGS, the half-thick absorption layer requires less deposition time, which can reduce energy consumption, labor costs, etc., and also increase throughput. However, we do not expect there to be a similar reduction in non-material costs. This is because any non-full-load operation or standby status between processes will lead to increased running hours and thereby higher utility and depreciation expenses. Here, the non-material cost for CZTS absorber deposition is assumed to be 60%-80% of the CIGS.

- **Sulfurization**

According to the material provider, the cost for sulfur is \$400/ton and \$14.22/kg for selenium[10]. After considering the thickness of both and the cost of selenization at \$4.21/m^2, the material cost of sulfurization is \$0.12/m^2.

There are multiple non-reactive steps in the sulfurization/selenization process, including sample transfer, vacuum, heating, and cooling, which will reduce the advantages of the thinner absorption layer. Therefore, the non-material cost of sulfurization is also set to 60% -80% of selenization. Besides, although low-temperature processes can reduce energy consumption, depreciation is the most critical cost for expensive RTP equipment, and lowering the temperature may take longer to achieve the same film thickness. As a result, the loss and gain are difficult to quantify, and the change is limited. Thus low-temperature sulfurization is considered to have the same non-material cost and increase the uncertainty from -30% to +60%.

- **Encapsulation**

CZTS on glass is assumed to have the same encapsulation method as CIGS on glass. For the flexible modules (C and D), unlike rigid module encapsulation, there is no broad consensus on flexible thin-film cell encapsulation. This may be because of limited manufacturers of flexible thin-film cells as well as their low scale. Advanced encapsulation technologies may help producers gain an advantage over the competition, resulting in higher opacity of the technology. Therefore, there are many possible methods to encapsulate flexible cells, and the various processes are quite different. Some production lines use ultra-high quality barrier layers to improve the lifetime and reliability. This data is usually inaccessible and inaccurate when extrapolating to high volume pricing due to its high cost and irregular distribution. From industrial experience, we assume a flexible encapsulation with ETFE + PET + TPO structure.

In similar encapsulation processes, materials account for about 90% of the total cost[1, 11]. Hence the non-material cost is considering 10% of the encapsulation expenses with 30% uncertainty.

Table S4. Assumptions in the marginal LCOE calculation

Assumptions	Note
Metal roof project with building material offset	This is the cost of stainless steel substrates.

\$4.8/m^2.	
Modules can work at rated efficiency.	To reduce the diversity of selecting different branded products.
Installation labor costs and supply chain costs are borne by the builder.	Through cooperation with building construction [12].
BOS and inverter costs are similar to residential rooftop photovoltaics. Assuming 50% of electrical components cost is area-related, 50% is power-related.	Data source:[13-15].
10% Profit margin; 4 Peak Sun Hours per day; 3% discount rate.	Basic assumptions.

Marginal LCOE calculation:

$$\text{LCOE}=\frac{\sum_{t=1}^{n}\frac{I_t + C_{investment}}{(1+r)^t}}{\sum_{t=1}^{n}\frac{E_t}{(1+r)^t}} = \frac{\sum_{t=1}^{n}\frac{C_{marginal}}{(1+r)^t}}{\sum_{t=1}^{n}\frac{E_t}{(1+r)^t}} = \text{Marginal LCOE}$$

$C_{investment}$: Capital expenditure, equals to marginal cost.

I_t: Operations and maintenance expenditures in the year t. Since there is no inverter replacement and in this case, and the inverter cost in terms of \$/W already considers all expenditures, this term is equal to 0.

r: discount rate.

n: expected lifetime of 25 years.

E_t: Energy generated in the year t, considering the annual performance decline of 0.8%.

The cost and price of stainless steel CIGS:

Since there is no available CIGS cost of stainless steel modules, we believe it follows the same pattern as CZTS, which is ~80% of the cost of glass modules. The retail price of commercial stainless steel CIGS is from Midsummer's products with high similarity, plus the same BOS and inverter cost to form the installed system cost.

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