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### 1. Introduction

Analysis of manufacturing cost and market niches for Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) solar cells<sup>†</sup>

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Thin-film solar cells, due to their low material usage and flexible substrates compatibility, have the potential to fill market niches for photovoltaic (PV) technologies. Among them, the Cu(In,Ga)Se<sub>2</sub> (CIGS) solar cell is a widely deployed mature technology. However, the usage of scarce material like Ga and In is considered a major hindrance for its further scaling up. The commercial opportunity of its promising counterpart Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) with a similar structure but low-cost potential, has not yet been fully recognized. In this paper, the bottom-up approach is used to build models of cost analysis for CZTS on the different substrates with their probability distribution simulated by the Monte Carlo method. The resulting production costs are \$41–52 per m<sup>2</sup>, making them economically attractive. Prospective strategies for further cost reduction are also suggested. The fundamental technical features of CZTS are reviewed, identifying the large efficiency potential of this PV technology. Analysis of different market opportunities is performed to fit the market demands better. Moreover, possible constraints and promising pathways towards the commercialization of the emerging CZTS technology are proposed.

With worldwide awareness of reducing carbon dioxide emissions and a growing appetite for clean energy, the annual installation of PV capacity has exceeded 100 GW in recent years.<sup>1</sup> Within the next decade, solar energy can potentially reach a total installed capacity of 10 terawatts.<sup>2</sup> In view of such large market size, it is likely that there will be diversification of PV technologies into market niches, and the full potential of PV technologies should be maximized.

Silicon solar cells have dominated the market due to their stable efficiency and rapid cost reductions. Thin-film products occupied nearly 10% of the solar market before 2015, witnessing a significant drop to around 5% with the recent decline in the price of silicon solar cells.<sup>3</sup> However, this still represents a steady increase in market volume for thin-film PV technology because the overall market size has increased so quickly, and this technology type should not be ignored. Unlike wafer-based solar cells, thin-film solar cell absorbers require only a few microns to absorb the desired spectrum due to their high light absorption coefficient. Thinner cell structure offers the prospect

of using flexible substrates, which brings a variety of possibilities for their future development.

CdTe is a commercially available thin-film PV technology with appreciable efficiency beyond 22% 4 and high market share.5 However, the incompatibility of cadmium with RoSH and the rarity of tellurium will eventually limit its large-scale deployment.6 The Cu(In,Ga)Se2 (CIGS) solar cell is another commercialized thin-film technology and has achieved a 23.3% laboratory efficiency.7 Nevertheless, the usage of scarce and precious metal Ga and In may limit its widespread application due to cost and supply constraints.8 To address these issues, the Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) solar cell, with a similar I2–II–IV–VI structure, has been developed as an alternative candidate to CIGS. CZTS is generally considered to have lower costs and reduced environmental impact due to its use of more abundant elements. However, no quantitative analysis has been conducted to evaluate the commercialization potential of CZTS. For photovoltaic technologies, emerging an early-stage manufacturing cost analysis can help clarify cost structure and identify key costs that need to be reduced to promote commercialization. Market analysis is also critical as it considers technology features in addition to cost that are valuable to end users. Technologies under development must identify market niches of sufficient size where they can reasonably expect a competitive advantage. Both cost and market studies help to guide the direction of research and development towards a product that can be commercialized.

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In this work: (i) a CZTS cost model is built to estimate the production cost of various CZTS product types and identify research paths to reduce this cost; (ii) the efficiency records and potential of CZTS, as well as the mechanism of efficiency deficit and feasible solutions, are reviewed; (iii) market analysis is conducted to identify potential market niches and related customer requirements for these CZTS products; and (vi) an assessment of the suitability of the CZTS product for each market niche is made, together with the investigation of technical and cost targets necessary for the CZTS product to be commercially competitive.

### 2. Cost analysis

The CZTS solar cell technology has not yet been commercialized on a large scale, making cost estimation very difficult. However, the CIGS technology, which has a very similar structure to CZTS, is currently in mass production by a number of companies.<sup>9</sup> During the commercialization of CIGS, several cost models have been built: Schuler *et al.* provided a detailed financial model containing manufacturing cost,<sup>10</sup> Kapur *et al.* highlighted the importance of improving process yield to reduce cost,<sup>11</sup> and Horowitz *et al.* further linked the module cost to manufacturing volume.<sup>12</sup> A CZTS manufacturing cost model can be built by adapting these existing bottom-up models.

Since precise values for the cost inputs are not readily available for high volume manufacturing of the CZTS technology, a Monte Carlo uncertainty approach was used to estimate the cost. In brief, data was collected from publications, price lists, and industrial communications. Each cost parameter has its own uncertainty based on the number and quality of each data source, so in the model, each parameter is assigned an uncertainty range based on our judgment. In the Monte Carlo analysis, each parameter is sampled N (N = 50~000 in this work) times from a probability distribution formed from the uncertainty range, and N different calculations of cost are obtained. The distribution of calculated cost indicates the range of possible manufacturing cost. In this case, there are significant uncertainties arising from (i) the progression of time since the referenced cost studies have been completed, and (ii) the cost of CZTS specific processes that are not yet commercialized. Further details about this model can be found in our previous work.<sup>13,14</sup>

#### 2.1 Process sequence

Four product types were analyzed: a glass–glass standard CIGS structure as a reference, and three alternate CZTS products on different substrates (Fig. 1). The detailed process sequences are provided below and in Table S1 (ESI†).

**Process A.** CIGS on glass – with process steps and recent cost data from ref. 12.

**Process B.** CZTS on glass – all process steps are the same as Process A with the exception of: (i) different absorber material and thickness of CZTS based on the current literature value, and (ii) sulfurization instead of selenization.

Process C. CZTS on stainless steel - a different substrate is used compared to Process B. This leads to three process changes: (i) impurities in stainless steel like Fe and Cr are detrimental for solar cells,15 so a 50 nm Ti layer is deposited directly on the stainless steel (SS) to block undesirable elements diffusing during the high-temperature processes, (ii) soda-lime glass is believed to supply Na during the device fabrication, which is beneficial for the grain crystallinity and overall device efficiency,16 so when using a steel substrate, a 10 nm additional sodium source layer (usually NaF17) is required to achieve acceptable device performance, and (iii) a flexible encapsulation configuration is needed to match the flexible substrate, here ethylene tetrafluoroethylene (ETFE) polyethylene +



Fig. 1 Structure diagram of process A-D. (a) CIGS on glass, (b) CZTS on glass, (c) flexible CZTS on stainless steel, and (d) flexible CZTS on plastic.

terephthalate (PET) + thermoplastic polyolefin (TPO) structure is used.  $^{\mbox{\tiny 18}}$ 

**Process D.** CZTS on plastic (PI) – compared to Process C, the additional Ti barrier layer is no longer needed because there are no impurities in the PI to block. However, the PI cannot withstand high temperatures, so a lower temperature sulfurization process is required.

### 2.2 Cost results

In this work, we implement a simplified cost model, where we divide manufacturing costs into two categories – material costs (including all input materials such as substrate material, sputter targets, and precursor gases) and non-material costs (including labor, electricity, equipment depreciation, and spare parts). In the referred detailed cost analysis, all the input data values are not provided,<sup>12</sup> so we use the cost results data (which was divided into materials, depreciation, labor, utilities, and maintenance) and adapt it to our simpler model. We take the cost values from that analysis and adjust them according to the expected differences in input costs. The cost assumptions are summarized in the ESI (Tables S2 and S3, and notes†).

After simulation by the Monte Carlo algorithm, the costprobability distribution of different processes is obtained. As shown in Fig. 2, Process A (CIGS) has the highest costs (using the \$ per  $m^2$  metric) among all the sequences listed, so the CZTS alternatives are expected to have lower area-based costs.

Process B has a cost reduction of about \$10 per m<sup>2</sup> (~16%) compared to A. It can be seen from the comparison between Fig. 3a and b that this is due to (i) the material cost of the CZTS absorber layer sputtering is reduced to a negligible level, which is because the use of abundant elements and the thinner layer, and (ii) the use of sulfur to replace selenium leads to a reduction in the cost of this process step.

Process C has the lowest cost of these four product types. In Fig. 3c, the cost of the stainless steel substrate is much lower than that of glass. The extra NaF and Ti layers required because of the application of stainless steel substrate do not add much



Fig. 2 Total module cost for different product types based on the assumption of 1 GW per year manufacturing volume.

cost due to these being such thin layers. Also, the flexible encapsulation avoids the addition of the heavy top glass and frame, leading to further cost reduction.

Process D is the highest cost one within these three CZTS products (Fig. 2). The high-temperature-resistant PI substrate is very expensive (Fig. 3d). There were only a limited number of suppliers found for such PI substrate, with a wide range of prices, so the uncertainty of this cost is also relatively high. Since this cost dominates, any attempt to achieve a low-cost plastic product would require a PI supplier with a very low cost or an alternative lower-cost plastic substrate.

The calculated results are compared with the cost or price of equivalent commercial products and show a little higher due to the development of the technology since the referred study in 2015.12 Commercialized glass-glass CIGS modules are sold between \$0.25 and \$0.30 per W,19 close to our cost estimate of Process A of \$0.33 per W if we assume the 18% efficiency (18.6% efficiency on 1 m<sup>2</sup> has been achieved<sup>20</sup>). Since the cost of CIGS has reduced by 10-25% compared to our estimates, this suggests cost improvements have been implemented since our referred study.12 It is possible that some of these improvements could also be similarly applied to the CZTS process, leading to an even lower cost than we have estimated above. In this study, we take the conservative approach of assuming that the CZTS cost is exactly what we have estimated. The manufacturing cost of a CZTS product on plastic substrate is \$0.35 per W reported by Crystalsol (a CZTS solar cell manufacturer from Austrian), although it is not clear from their report whether it is a full module or just the cell.<sup>21</sup> Our estimate of CZTS on the plastic substrate (process D) is \$0.52 per W with 10% efficiency, which is much higher than the value that Crystalsol reported. This could be due to the difference in module cost or also because Crystalsol uses a very different roll-to-roll process with a different cost structure. There is no commercial product similar to process B and C for reference. However, it should follow the same trend as the manufacturing cost, *i.e.*, lower than the cost of D.

### 2.3 Strategies for cost reduction

The manufacturing cost and module efficiency together determine the cost in dollars per watt (\$ per W), which is another important metric to consider and minimize. Under 1 sun condition (1000 W  $m^{-2}$ ), it can be derived from manufacturing cost (\$ per m<sup>2</sup>) and efficiency. The current efficiency of CZTS solar cells on glass substrates is slightly above 10%,22 and hence we assume a 10% module efficiency for CZTS. At this efficiency, the manufacturing cost of \$51 per m<sup>2</sup> corresponds to \$0.51 per W, which is quite high. It can be improved by reducing the manufacturing cost and increasing efficiency. Horowitz et al. discussed improving efficiency usually lead to an increased manufacturing cost.<sup>12</sup> Peters et al. suggested that some options exist where the improvement in efficiency is worth pursuing, even with a higher cost per module.23 Kapur et al. proposed lower-cost process options, which could still maintain the efficiency (e.g., improving process yield or removing the frame).11 The impact of these strategies is shown in Fig. 4a. Assuming



Fig. 3 Cost breakdown with uncertainties for sequences A–D. (a) for CIGS on glass, (b) for CZTS on glass, (c) for CZTS on steel, (d) for CZTS on plastic. The thinner line in each sub-cost presents the upper and lower limits of the cost due to uncertainty.

that the manufacturing cost (per module) is unchanged, increasing the efficiency from 10% to 15% will reduce the costs by approximately a third.

However, the related processes for high efficiency will likely be more expensive than the ones we have modeled.<sup>24</sup> Some work has been done suggesting the increase in manufacturing costs due to the efficiency improvements can be offset in the long term.<sup>12,23</sup> The impact and trade-off of such changes can be assessed using the cost results presented here. For example, considering the thickness of the absorber, which is typically 0.75  $\mu$ m currently. The current CZTS effective collection length of less than 1  $\mu$ m suggests that the absorber thickness should not exceed 1  $\mu$ m for the proper carrier collection,<sup>25</sup> and a thicker absorber layer has a limited contribution to improving efficiency.<sup>26</sup> However, with improvements in material properties such as lifetime and diffusion length, a thicker absorber may be required to achieve higher efficiency. If, for example, higher efficiency requires a doubling of the thickness of the absorber,<sup>27</sup>

an estimate of cost increase can be made. Doubling the thickness would not double the cost of the CZTS sputtering step and the sulfurization steps: the material usage would likely double, but the equipment depreciation (which dominates the cost) would not double because the equipment could be optimized for this layer thickness (for example increasing the number of sputter targets). We would therefore expect the cost to increase by less than \$5 per m<sup>2</sup>, and this additional cost would still need to be justified by the additional efficiency gain. In addition, improving the process yield from 90% (assumed in CIGS reference data) to 95% can also contribute to the cost reduction. Although the effect is not as significant as improving efficiency, it is still a feasible approach to reduce the cost.<sup>28</sup> Frameless structure offering \$7 per m<sup>2</sup> benefits (\$0.05 per W), the practicality of which still needs to be studied, and there may be a negative impact of Balance of Systems (BOS) costs need to be accounted for.



Fig. 4 (a) Strategies for cost reduction in \$ per W; (b) record efficiencies of each technology at different cells per module area.

Different markets seek PV modules with different sizes, and solar modules suffer from decreased efficiency when scaling up to large areas, which may lead to additional cost to control the uniformity when producing large modules. Fig. 4b plots the effect of solar cell per module size on efficiency from the literature,29 with the addition of Dye-Sensitized Solar Cell (DSSC), CZTS, and amorphous silicon (a-Si) data. The efficiency of crystalline silicon (c-Si) remains above 25% over a wide range of module sizes. Amorphous Si almost keeps the record efficiency at around 10% in large-area production. Perovskite solar cells suffer the most obvious performance decline, with efficiencies from 25.2% on an area of approximately 0.1 cm<sup>2</sup> to less than 15% on a module level.<sup>20,29</sup> Both CIGS and CZTS, which are similar technologies, lose around 10% with every 10-fold increase in area. Although CZTS exhibits an acceptable efficiency trend, research on large-area uniformity and stability also needs to be progressed to avoid additional costs.

### 3. CZTS technology features

CZTS solar cells can be fabricated in different configurations, achieving different efficiencies. Here we outline some of the important achievements to date, as well as the efficiency potential for CZTS.

#### 3.1 CZTS on glass

Selenium-containing CZTSSe solar cell has achieved world record efficiency of 12.6%, and pure sulfide CZTS has recorded laboratory efficiency of 11% on 0.24 cm<sup>2</sup> area, and 10% on 1 cm<sup>2</sup>.<sup>22</sup> This particular configuration is most similar to the standard c-Si technology (flat plate, inflexible, relatively heavy) and so would need to compete head-to-head against other rigid PV products.

### 3.2 Flexible CZTS on plastic

An Austrian CZTS manufacturer, Crystalsol, has achieved an efficiency of 9.5% on a polymer substrate  $(0.034 \text{ cm}^2)$  and 7.5% on a module level (400 cm<sup>2</sup>) by using single-crystalline technology.<sup>30,31</sup> This configuration, being flexible, has the advantage of high production volume by roll-to-roll manufacturing and

wide applications due to the applicability on curved surfaces. It is also much lighter due to the removal of the heavy glass–glass encapsulation.

### 3.3 Flexible CZTS on steel

A 10% efficient CZTS solar cell has been achieved (0.5 cm<sup>2</sup>) using flexible Molybdenum foil, which is currently the highest efficiency using metal substrates.<sup>32</sup> In 2018, UNSW achieved an efficiency of 6.2% on 0.24 cm<sup>2</sup> stainless steel substrates,<sup>33</sup> and there is a high potential to transfer some of the strategies for recent improvements in CZTS on the glass to increase the efficiency in the future. This technology is both flexible and robust, with high mechanical strength and corrosion resistance.

The efficiency potential for CZTS is promising not only because of its high detailed balance limiting efficiency of over 30% <sup>34</sup> but also due to the identification of the limiting factors for the efficiency improvement and the fast development of this technology in R&D. Possible origins for the low efficiency of CZTS include (i) deep intrinsic defects like SnZn, acting as midbandgap recombination center. This will lead to short carrier lifetime and severe bulk recombination;35,36 (ii) unfavorable heterojunction band alignment. The traditional CdS buffer layer is criticized for forming a "cliff-like" Conduction Band Offset (CBO) with CZTS, which facilitate the interface recombination, contributing to Voc deficit;37 (iii) band tailing issue due to the cation-disordering defect clusters like [2CuZn + SnZn] and [2VCu + SnZn], resulting in bandgap fluctuations;38 (iv) secondary phases contribute to serious interface recombination at CdS/CZTS and CZTS/Mo interface;39 (v) bulk inhomogeneities due to the narrow phase stability.40 However, multiple approaches have been proposed to overcome the above problems. Cationic substitution can be used to reduce the antisite defects and disorder.41 Different buffer layers have been developed in order to provide a more favorable spike-like band alignment<sup>42</sup> as well as Cd-free processes. Postdeposition treatment with alkaline elements is also an effective method and has been successfully implemented in CIGS.43 The evolutionary history of CZTS is only twenty years.44 Compared with the forty years of CIGS, it is undoubtedly a young technology.45 And considering the similar material properties and development

roadmap to CIGS, CZTS is highly anticipated to reach a similar level of efficiency as CIGS.<sup>24,46</sup> For the purpose of the market analysis, we analyze the market options that would be available if we are able to successfully improve the efficiency of the CZTS technology to match that achieved by its sister technology CIGS.

### 4. Potential market analysis

Each market segment for PV products may value certain characteristics differently, such as cost, efficiency, weight, and flexibility. Alternative PV technologies differ in these characteristics, and a particular combination of these factors may be well suited to particular markets. In order to competitively enter a certain market, new technology must be more attractive when compared with the current market leaders as well as with other potential entrants. In cases where technology has both advantages and disadvantages compared to the alternatives, it is possible that further development can address or solve the negative factors and further enhance the positive factors. This understanding thus lead to research and product development parties focus on developing towards the most effective product for each market.

CZTS products have the following features (that will be described in more detail later) that could make them appealing in certain markets:

(i) Ability to be scaled to terawatt (TW) levels – it is a technology that only uses earth-abundant elements that can be easily scaled up to match the increasing PV market;

(ii) Voltage – monolithically-integrated thin-film solar cells like CZTS can easily be configured for higher voltages than c-Si modules for the same module area, which can be important in some applications.

(iii) Low light performance – CZTS cells have a good low-light response, enable gaining additional energy in cloudy days or indoors.47

(iv) Weight and flexibility – CZTS modules can be configured with low weight and high flexibility, making it usable in a wider variety of applications and reducing the structural strength requirements for the mounting structure.

(v) Long-term durability – CZTS solar cells tend to have longterm functionality and efficiency similar to commercial technology CIGS due to their structural similarity.

Any technology, with its particular mix of advantages and disadvantages, may have a market niche particularly suited to it. From the features of CZTS identified here, we have identified a number of market segments where we believe a CZTS product could show promise or compete in. For each market niche, we discuss possible alternative PV alternatives, including commercialized technology and other potential entrants, and consider the potential for CZTS to compete successfully against them.

### 4.1 Market opportunity for CZTS in rooftop PV

Rooftop PV accounted for about a quarter of installed photovoltaic capacity in 2018, at 27.9 GW.<sup>48</sup> And different predictions indicate that the compound annual growth rate will be around 10% in the next five years.<sup>49,50</sup> Crystalline silicon has accounted for about 90% of the traditional rooftop photovoltaic market, with a-Si, CIGS, and CdTe occupying the remaining market with roughly equal market shares.<sup>3</sup> Therefore, the market for CZTS and other thin-film PV technologies is around 5 GW per year. When considering the commercial application of CZTS, it is worth considering such existing large markets, with its potential for a larger volume of sales. In addition, exposure and demonstration of new technology can help it gain recognition and acceptance with consumers with flow-on effects to other market niches.

Rigid CZTS with a glass substrate is first chosen for this market analysis due to its similarity with other main competitors like c-Si with rigid glass that dominates this market. In this market, we also consider the potential for a lightweight flexible configuration (CZTS on PI) since it may open up another segment of the rooftop market.

• Efficiency. The efficiency of a solar cell represents the device's ability to convert sunlight into electricity through the photovoltaic effect. Higher efficiency will result in more electricity generation per unit area, which is especially important for space-constrained situations. Also, much of the cost of the balance of systems (wiring, installation labor, *etc.*) is closely related to the total area of the PV array, so higher efficiency will generally lead to lower Levelized Cost of Energy (LCOE).

The efficiency of most installed c-Si, CdTe, and CIGS modules on the market is between 15-20%,<sup>51,52</sup> while the efficiency of existing CZTS products is only 7.5%.<sup>30</sup> Unless the CZTS technology can reach its efficiency potential, this low efficiency will limit the benefits of its low-cost (\$ per m<sup>2</sup>) in comparison to its competitors.

• Ability to be scaled to TW levels. As the installed capacity of photovoltaics is reaching the terawatt scale and will continue to increase, abundant raw materials will be a prerequisite for any PV technology to capture a significant amount of this market. Also, easily controlled and highly repeatable processes are beneficial for mass production to reduce the cost of quality control and the demand for skilled labor, as well as increasing the manufacturing yield.

C-Si PV technology has an installed base of hundreds of GW, made possible by the abundance of silicon. Ga and In in CIGS are rare and therefore expensive, which is considered as unsuitable for similar large-scale deployment.53,54 Tellurium in CdTe is one of the least abundant elements,6 which is also required by many other industries and has inherent supply chain risks.55 In addition, PV technology with cadmium as the main component is not desirable due to health and safety concerns. The European Commission prohibits electrical and electronic equipment with a cadmium concentration exceeding 0.01%,56 which also limits the development of CdTe. In contrast, the CZTS cells with earth-abundant elements can avoid being restricted by raw material supply and high prices. From the manufacturing perspective, the CZTS materials are all non-toxic, avoiding toxic leak detection and control costs during manufacturing. The use of vacuum sputter processes which have been continuously developed and widely used in the industry<sup>57</sup> can ensure high repeatability, high film uniformity,

and accurate thickness control in mass production. Thereby, CZTS solar cells have no barriers to TW level scaling.

• Module cost. Module cost is a significant fraction of the total expenditure of a PV system, so its cost (in \$ per m<sup>2</sup>, or when combined with efficiency in \$ per W) will impact the economics of the system. Our cost analysis above, which is adapted from data from a 2015 NREL study,<sup>12</sup> shows that CZTS at 1 GW year<sup>-1</sup> production volume would cost \$0.51 per W with 10% efficiency. In the same year, the cost for c-Si was estimated at \$0.74 per W by NREL using a similar cost model,<sup>58</sup> and market analysis suggested that a selling price of \$0.6 per W is needed for CZTS to be competitive.<sup>59</sup>

Since 2015, the cost of PV modules continued to decline with the development of each technology and economies of scale. CdTe demonstrated a slightly more than \$0.3 per W module cost in 2017.60 The cost of c-Si was \$0.3 per W in late 2019,1 and the cost of CIGS was \$0.25 per W in 2018.61 If CZTS also has a 16% cost reduction as happened in CIGS, then the cost should be \$0.41 per W at 10% efficiency. Since the cost of power generation is extremely dependent on the efficiency of the modules, assuming 18% efficiency potential can be demonstrated, the cost of CZTS will be reduced to \$0.23 per W, similar to the alternative technologies. These estimates are based on 1 GW year<sup>-1</sup> production, and further expansion to larger production volumes would lead to further cost reductions.62 In addition to this theoretical analysis, a \$0.35 per W cost of the CZTS module was achieved in 2018 by the company Crystalsol using a flexible roll-to-roll process.21

• Weight. Heavier modules put more load on the roof, which may not have sufficient strength to support, such as common commercial membrane roofs. Moreover, the installation costs of a lightweight module can be 10% lower compared to that of a standard module<sup>63</sup> due to the reduced use of mounting material and lower labor costs resulting from a simpler installation process.

As a minimum to compete in this market, a PV product needs to be at a similar weight with standard c-Si modules used today – typically 15–17 kg m<sup>-2</sup>.<sup>64,65</sup> Lighter weight than this would provide additional market value. Rigid thin-film solar modules can be lighter than this, at 12 kg m<sup>-2</sup>.<sup>66</sup> However, if the glass is replaced with a lightweight and flexible encapsulation, the module weight can be as low as 1.7 kg m<sup>-2</sup> (0.15 lb per ft<sup>2</sup>).<sup>67</sup> According to our cost calculations, such a lightweight configuration could be achieved by the proposed CZTS product with PI substrate, at a slightly higher cost than the rigid glass product.

For this type of application, the CZTS product would be competing against other similar flexible, lightweight options such as other thin-film technologies or c-Si with lightweight encapsulation. In making the comparison with those competitors, the lighter products would have access to more roofs, and the product with the lowest cost (\$ per W) would also be favored. Based on currently available information, the CZTS option (if the efficiency potential can be realized) would be attractive in cost and efficiency compared to other thin-film products, and its weight would give it an advantage against semi-flexible c-Si products<sup>68</sup> since these silicon solar cells still need to be thick enough for complete absorption, which will inevitably affect their flexibility and weight.

 Assessment of CZTS opportunity in the traditional rooftop PV market. The rooftop PV market is huge and still developing, which makes it a very important market for a new PV technology to consider (Table 1). In rooftop applications where weight is not a critical issue, however, CZTS will struggle to compete in cost and efficiency with c-Si. There is an opportunity for CZTS to compete in applications where it has an advantage over c-Si, such as those valuing or requiring a lightweight product. Significant reductions in BOS installation can be achieved using lightweight photovoltaic (LPV) systems, and about 40% of commercial rooftops are not suitable for traditional PV arrays because of weight.63 The total market size where CZTS lightweight products have a competitive advantage is quite small (only very weak roofs, which are 11% of the commercial rooftops<sup>63</sup>), which limits its attractiveness, but it does represent a potential market niche for the CZTS technology.

In the weak roof market, CZTS would be competing against other thin-film technologies that are able to be fabricated on lightweight substrates such as CIGS. This presents a market barrier for CZTS, since supply chains and market channels that would need to be developed for a new entrant. Also, CZTS must compete in efficiency and cost against other thin-film PV technologies that share the lightweight advantage. It requires CZTS to increase efficiency from the current level of 7.5% to match CIGS (18%) using lightweight configuration.<sup>21</sup> Achieving this efficiency would also increase its competitiveness against CdTe, which has an additional disadvantage of unfavorable elements.

#### 4.2 Market opportunity for CZTS in IoT

The "Internet of Things" (IoT) is a concept where a large number of sensors are distributed, each with perception-

 Table 1
 The summary of the comparison between CZTS and other technologies in the traditional rooftop PV market. \*CIGS could also use lightweight flexible substrates

Feature	c-Si	CIGS	CdTe	CZTS (glass)	CZTS (PI)
Efficiency	1	1	1	X (at present)	<b>X</b> (at present)
Ability to be scaled to TW levels	1	X	×	$\checkmark$	$\checkmark$
Module cost (\$ per W)	1	1	1	X (at present)	X (at present)
Weight (strong roof)	1	1	1	✓	✓
Weight (weak roof)	×	<b>X</b> *	X	×	1
Key issue	Not suitable for some commercial roofs	Usage of Ga and In	Cadmium containing products are restricted	Needs to achieve efficiency potential	Needs to achieve efficiency potential

transmission-intelligent processing. Its potential applications in industry, agriculture, security, and other infrastructure fields have promoted the rapid development of this field. By the end of 2020, billions of IoT devices are expected to be utilized.<sup>69</sup> To enable this, there is a need to identify the best method of powering these devices. Because of the large number and wide distribution of these devices, as well as the impracticality or expense of replacing batteries in some application scenarios, it is appealing to design self-powered devices. Solar energy has the highest energy density compared with other ambient energy sources,<sup>70</sup> and PV is a proven technology, hence a promising approach to power IoT devices.

Streetlights and water quality monitors are examples of the successful combination of IoT and PV technology.<sup>71,72</sup> This kind of application primarily requires PV modules with high efficiency, durability, and reliability; and has few restrictions on weight, flexibility, or other properties. Thin-film solar cells have also recently attracted the attention of academia due to the economic applicability and good low-light response.<sup>73,74</sup> However, most commercial PV-powered IoT applications are still in the development stage.

CZTS on stainless steel and plastic are both promising for this application due to their lightweight and flexible features. The former is cheaper and robust, while the plastic-based device is more flexible, allowing it to be used for various configurations of IoT devices. We now compare the features of CZTS products to crystalline silicon technology as an existing competitor in IoT applications<sup>75</sup> as well as the low-cost candidates, DSSC, and a-Si cells, which have also been explored in IoT applications.<sup>76,77</sup>

• Efficiency. Different IoT devices and applications have different energy requirements. The power usage of most sensors is in the range of 100  $\mu$ W to 1 mW, which results in several milliwatts hours of power consumption per day, depending on the working time.<sup>78</sup> The power rating of a PV module required for any particular application will also depend on the incident light intensity and duration, as well as the availability of battery storage. If there are also area constraints on the PV module, the minimum cell efficiency requirement can also be derived. Since these factors vary significantly between applications, there is no universal PV cell efficiency requirement for IoT devices. However, higher efficiency PV technologies will be able to service larger segments of the market by being able to provide sufficient power with a smaller available area or under lower lighting conditions.

Due to the current low-efficiency, CZTS is more likely to compete well in applications with high light energy such as outdoors in full sunlight. At 1 sun light intensity(100 mW cm<sup>2</sup>), even 1 cm<sup>2</sup> solar cells can generate about 10 mW h within 1 hour, which can meet the daily energy required for IoT devices. For the more challenging indoor applications, experiments have confirmed that solar cells at 10% energy conversion efficiency can meet the needs of some IoT devices.<sup>74,79</sup> Crystalline silicon, DSSC as well as a-Si modules are able to meet this 10% efficiency requirement. The current efficiency of CZTS cells on plastic and stainless steel is 9.5% on 0.034 cm<sup>2</sup> and 6.2% on 0.224 cm<sup>2</sup> respectively.<sup>21,33</sup> The next step is to increase the efficiency a little bit and scale up to larger cell and module sizes.

• Long-term durability. For IoT applications requiring a long service life, the PV power source must have a suitably long lifetime without significant power degradation. Any PV technology that is susceptible to degradation will be at a significant disadvantage.

A study shows the actual power of deployed a-Si modules decline 30% during the first 1.5 years and then stabilized, which means that the efficiency for most of the operational life is lower than the as-produced efficiency.<sup>80</sup> The stability of DSSC has also been one of its most pressing issues,<sup>81</sup> dropping 32% with irradiation and more than 50% with heating in 1.5 months.82 In comparison, flexible CIGS modules commercialized on a large scale are sold with a 5 year workmanship and a 25 year performance warranty (80% power after 25 years<sup>83</sup>), comparable to that of silicon cells. Moreover, the measurement results also proved that the CIGS modules manufactured before 1988 still maintain 91% power after ten years under Standard Test Conditions (STC).<sup>84</sup> The durability performance should be better with the advancement of technology developed over time. Although durability studies have not been carried out on CZTS modules, their similarity to CIGS suggests that they would be similarly durable.

• Physical properties (weight, flexibility). With the trend of miniaturization and reductions in the weight of IoT hardware,<sup>85</sup> there are further restrictions on the allowable weight, size, and other physical properties of the solar cells. Solar cells with glass substrates will add significant weight, and not every IoT device can carry flat, brittle glass. In many cases, we would expect that lightweight and/or flexible cells would be more attractive because of the reduced weight load and providing a wider range of physical design possibilities for the IoT device.

Silicon, as an indirect bandgap semiconductor, usually requires a thicker active layer to achieve complete absorption, resulting in rigid cell and heavier encapsulated modules. CZTS and other thin-film cells can benefit from thinner modules, as well as lightweight, flexible substrates and encapsulations.

• Voltage. Since PV power generation is intermittent, most PV powered IoT devices will require an energy storage device, such as a battery, to allow for periods of low light. However, the maximum power point voltage ( $V_{\rm mpp}$ ) of the solar module needs to exceed a certain threshold value in order to charge the battery. This can be particularly challenging under low light conditions. Failure to match appropriate  $V_{\rm mpp}$  with the battery may result in the need to use a step-up converter. This requires additional electronic devices while causing power losses during the conversion process. For this reason, solar modules with higher  $V_{\rm mpp}$  may be favored in some IoT applications. Higher  $V_{\rm mpp}$  can be achieved by series-connecting multiple solar cells into a module.

Thin-film technologies such as CZTS are usually manufactured in a way that connects many sub-cells together in series to form a "monolithically integrated" module. This reduces process complexity during the manufacturing process,<sup>86</sup> and more importantly, allows relatively high module voltages to be easily achieved. This is helpful for IoT applications where high voltages are needed but only a small area is available for the

solar module. For example, a 2 cm  $\times$  2 cm CZTS module can be fabricated with a V<sub>mpp</sub> more than 1 V by series connecting two or three cells.<sup>22,87</sup> In contrast, c-Si cells are typically made as single cells of area 244 cm<sup>2</sup> with about 0.5 V open-circuit voltage, making obtain such a high voltage would require cells to be cut into smaller pieces and soldered together in series, which would be much more complicated to achieve.87 Although it is feasible to utilize booster circuits to power IoT devices with small-size solar cells, up to 30% energy could be lost due to the voltage up-conversion.88 Hence, for small or single-cell IoT devices, if the energy storage system is considered, then the voltage will be the deal-breaker. Thin-film PV technologies with monolithic integration will therefore have a competitive edge.

• Low light performance. In outdoor conditions, good lowlight performance of solar modules helps to obtain more energy in the morning and evening, thereby reducing the system's dependence on energy storage. In addition, this merit also has the significance of improving applicability in indoor environments with poor light conditions. Generally, the available indoor light energy density is about 1% of outdoor, and the spectral range of the LED is between 400-800 nm.70,89 Low energy density and narrow spectrum range together increase the power generation requirements for the PV component. Hence, solar cells for this application must have excellent poorlight performance (typically high shunt resistance<sup>90,91</sup>), together with sufficiently large areas in order to meet the demand in an indoor environment.

Compared with crystalline silicon cells, thin-film solar cells are considered to have better weak light performance and spectrum response, resulting in a higher proportional efficiency being retained.<sup>90</sup> Specifically, a-Si has no obvious efficiency decline in a low light environment.90 A recent study from IBM showed that CZTS solar cells achieved 10% efficiency at lowlight, while the c-Si demonstrates only 4-9% efficiency.47 Furthermore, CZTS with tunable bandgap has the potential to work better indoors with a higher ratio of blue light by alloying or altering the ratio of elements,78 demonstrating the potential for border applications.

• Module cost. The concept of IoT is to use a large number of sensors to communicate data, and the core objective is to improve the performance of products through intelligent control. The cost of the IoT power supply must be compatible with the business case for each device. Since billions of sensors are envisioned, a low-cost PV component would likely be required. There are currently few applications in this market, so a definitive cost target for the PV system is not clear. However, if PV does get incorporated into IoT devices, the lower-cost alternatives are more likely to be selected, as long as they meet the other requirements outlined above.

The cost of DSSC is \$50–140 per m<sup>2</sup>,<sup>92</sup> which is \$0.4 per W to \$1.2 per W with its best efficiency of 11.9%.93

However, if it retains only 50% initial efficiency after 1.5 months,<sup>82</sup> the cost will be doubled then, which is unattractive. From our analysis, CZTS with plastic and steel has a manufacturing cost of \$52 per m<sup>2</sup> and \$41 per m<sup>2</sup>, respectively. A similar cost of \$57 per m<sup>2</sup> <sup>94</sup> is demonstrated by a-Si. If it could achieve 10.2% stabilized efficiency, CZTS on plastic and

Table 2 The summary of the comparison between CZTS and other technologies in the IoT market

Feature	c-Si	DSSC	CZTS (flexible)	a-Si
Efficiency	<i>」</i>	1	1	1
Long-term durability	1	X	1	X
Weight, flexibility	×	1	1	1
Voltage	X	1	1	1
Low light performance	X	1	1	1
Module cost (\$ per W)	1	X	1	1
Key issue	Heavy, low voltage, and poor low-light performance	Instability and higher cost	_	Degradation

steel is competitive with a-Si in \$ per W at 9.3% and 7.3%, respectively.

• Assessment of CZTS opportunity in this market. The projected billions of IoT devices could become a huge market for solar cells. However, the large-scale deployment of solar-IoT devices depends on the development of the IoT industry itself, and the wide use of solar cells for power. When the Internet of Things is no longer a concept product, and with an extensive application, diverse energy supply methods will be widely explored. The miniaturization of IoT devices means more flexible, and lightweight options are required, which makes thinfilm options preferred. Each technology has a unique situation. Taking all these aspects into consideration, flexible CZTS with high cost-performance, available materials, and good compatibility with small IoT devices is a promising choice compared to the other thin-film technologies (Table 2).

Due to its success in the traditional PV field, crystalline silicon may be more likely to be favored in applications without size and weight requirements, or without high voltage requirements. Also, if the stabilized efficiency is still satisfactory with low-cost, maybe the a-Si can also meet the requirements. For future development, stabilizing the process on flexible substrates and increasing the efficiency of CZTS can further increase the market competitiveness. And the long-term durability of CZTS also worth to be explored in addition to theoretical results.

#### 4.3 Market opportunity for CZTS in stainless steel roof BIPV

In recent years, there has been a pursuit of zero energy buildings in countries and regions, especially in the European Union, where corresponding legal provisions were promulgated to speed up the process.95 More and more builders and their partners are exploring the possibility of using Buildingintegrated photovoltaics (BIPV) to help achieve this goal. Parallel to this, the increasing PV industry size, and the related cost reductions and technology maturity have flow-on effects on improving the economics of BIPV.

The concept of BIPV is to replace traditional building material with PV products while remaining the same architectural function,<sup>96</sup> which means removing the BIPV components will cause the incomplete function of the building exterior. In practice, BIPV products include (i) Products that completely replace part of the building structure, such as solar tiles, which is already commercialized;<sup>97</sup> (ii) Tightly attached BIPV modules to existing roofs with a simple installation method such as peel-and-stick.<sup>98</sup> Although it looks like BIPV, it is actually Building-Applied PV (BAPV) since it is not architecturally functional. BIPV is either (i) or (ii), and we consider both here.

Roof-integrated BIPV occupies more than 80% of the BIPV market,<sup>99</sup> and we propose stainless steel is an interesting submarket of roof BIPV. CZTS with stainless steel is the most suitable configuration in this market due to the flexibility and compatibility. We compete in this segment and compare against other options on steel. Commercialized CIGS is the most obvious competitor, organic PV (OPV) and a-Si with stainless steel are also potential entrants from the literature.<sup>100</sup> Some features of importance, such as low-light performance, are very similar between the CIGS, CZTS, and a-Si (and are discussed in earlier sections). However, three features that are worth considering in detail, which will influence the investment and return of the PV system, are explored below.

• Energy output during the lifetime. Solar modules should have a promising efficiency and a durable lifetime to maximize the total energy output. BIPV can be considered as another form of PV array, and high-efficiency products are more attractive due to the feasibility of approaching zero-energy buildings. In addition, PV modules should have a long lifetime and maintain a high proportion of rate power.

The efficiency of the best OPV module is around 12%.<sup>20</sup> However, it is susceptible to water, oxygen, and even ultraviolet light, typically with an undeniable lifetime of fewer than five years.<sup>101</sup> The stabilized efficiency of a-Si is slightly above 10%.<sup>20</sup> Although it is higher than the current 7.5% efficiency of CZTS, the maximum theoretical efficiency of 15% limits its further development.<sup>102,103</sup> For CZTS and CIGS, neither efficiency degradation nor efficiency potential is a critical issue, as discussed earlier.

• Module Cost (\$ per m<sup>2</sup>). The module cost of CZTS, CIGS, and a-Si are very similar, ranging from \$41–61 per m<sup>2</sup> (as discussed before). The manufacturing cost of OPV is \$86–211 per m<sup>2</sup>,<sup>100</sup> which is quite high.

Since the system cost also includes the BOS cost and material offset in BIPV application, the economic applicability of the system cannot be obtained by simply comparing the cost of PV modules. Furthermore, the energy output and system cost interact with each other, and a combined metric of marginal LCOE is proposed and explained below.

• Marginal LCOE. Since a BIPV product has more purpose than simply electricity generation, its cost comparison is not just the electricity generated (*e.g.*, LCOE). For example, the cost of a structural PV product should be compared to an equivalent structural product in addition to considering the electricity generation. A proposed metric for this comparison is the Marginal LCOE. This is calculated by first determining the "Marginal cost of PV" – the additional cost of the BIPV product compared to the non-PV equivalent product (eqn (1)). Then, Marginal LCOE can be calculated by eqn (2). Assumptions can be found in Table S4<sup>†</sup> and notes.

Marginal cost 
$$C_{\text{marginal}} = C_{\text{module}} + C_{\text{BOS}} - C_{\text{alternative}}$$
 (1)

Marginal LCOE = 
$$\frac{\sum_{t=1}^{n} \frac{C_{\text{marginal}}}{(1+r)^{t}}}{\sum_{t=1}^{n} \frac{E_{t}}{(1+r)^{t}}}$$
(2)

Fig. 5a shows the marginal cost of CZTS with the breakdown. Some costs are area-related, including PV modules, material offset, installation, and electrical components, while others are power-related, such as inverter and electrician. Only arearelated costs contribute to cost reduction with increasing efficiency.<sup>23</sup> The system cost can be reduced due to the material offset and no installation cost when the integration is developed in the factory. However, the benefit of material offset is not very obvious, which is due to the low cost of the substrate. Installation costs are also presented and should be taken into account when modules are sold separately.



Fig. 5 (a) The marginal breakdown cost of CZTS at different module efficiencies (with and without installation cost); (b) the marginal LCOE of CZTS, CIGS, CIGS commercial products, and retail electricity.

Table 3 The summary of the comparison between CZTS and other technologies in the stainless steel roof BIPV market

Feature	a-Si	CIGS	CZTS	OPV
Energy output during the lifetime	1	1	1	×
Cost	1	1	1	X
Marginal LCOE	×	1	To be 🗸	X
Key issue	Limited potential efficiency	—	Improve efficiency	Low lifetime

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Fig. 5b shows the marginal LCOE for CZTS and CIGS, as well as the price of CIGS commercial products and retail electricity for reference. It suggests that CZTS will achieve the same marginal LCOE as CIGS once the efficiency is increased to around 15%. There are only a few CIGS products for reference, and the price is based on the 10 kW system. The incompletely established market and low-scale purchases together result in selling prices far higher than manufacturing costs. Moreover, the marginal LCOE for CZTS is also lower than the retail electricity price in the US,104 showing high attractiveness. The marginal LCOE of a-Si and OPV is obviously uncompetitive and hence not calculated. The manufacturing cost of a-Si is \$57 per m<sup>2</sup>, slightly higher than CZTS at \$41 per  $m^2$ , indicating a higher efficiency target to compete with CIGS. However, it is impractical due to the theoretical efficiency limitation of 15%. Also, the lifetime of OPV is typically less than two years<sup>105</sup> compared with 25 years of CIGS and CZTS, resulting in more than 1000% LCOE even with no degradation (optimistic).

There are other LCOE calculations for BIPV in the literature,<sup>106-110</sup> which give widely different LCOE values for technologies such as \$59 per MW h <sup>108</sup> and \$165 per MW h <sup>109</sup> for CIGS, and \$40 per MW h <sup>106</sup> and \$90 per MW h 110 for c-Si. They only consider LCOE rather than marginal LCOE, which may be more suitable for BAPV without cost offset rather than BIPV. It should be noted that the calculation of LCOE is affected by financial assumptions, and it is not easy to determine the best technology from an LCOE perspective by simply comparing LCOE calculations for alternate technologies that are reported in the literature since the assumptions are so different.

• Assessment of CZTS opportunity in this market. Roof BIPV application takes the largest segment in the BIPV market, and it is considered to have an impressive 29% compound annual growth rate,<sup>111</sup> making it an attractive market. The stainless steel configuration CZTS can be filled in the stainless steel roof BIPV, reducing the impact on the roof structure and function while enhancing the robustness of the PV module (Table 3). In the future, the use of non-solar grade steel can further reduce costs and improve economic feasibility.<sup>100</sup>

This market segment has not yet been fully established, and the current major participant is CIGS. Other competitors, such as OPV and a-Si are mainly troubled by efficiency improvements and stability, which restrict their energy output. In order to match the sister technology CIGS in terms of cost performance, CZTS on stainless steel needs to increase the efficiency to 15% to match the marginal LCOE.

### Conclusion

We have calculated the cost of three CZTS products using a Monte Carlo cost model and previous CIGS cost analysis data. At a production volume of 1 GW per year, the manufacturing cost of CZTS for different substrates is between \$41–52 per m<sup>2</sup>. The glass substrate configuration can cost less than \$0.3 per W at an efficiency of 15%. Further cost reductions are likely to be achieved by reducing depreciation of equipment and material costs through mass production. Given the similarity between CZTS and the already commercialized CIGS technology, and the expectation that efficiency limits are similar, we therefore would expect that with sufficient R&D to achieve these efficiencies, the cost in \$ per W will be improved compared to CIGS.

In considering market niches, we first identified the technical features of the CZTS technology that might be valued in different markets. We then selected three promising market niches and evaluated the potential for a fully developed CZTS technology to compete in these. In the traditional rooftop PV market dominated by crystalline silicon (with a large market share and significant economies of scale), there is a high barrier to entry for a new product such as CZTS. However, for the "weak roof" segment of this market, such as commercial membrane roofs, CZTS needs only compete with other thin-film products, where it might survive if the price-performance ratio is attractive. As for the IoT market, CZTS with plastic and steel substrate both have good prospects owing to its low weight, flexibility, and high voltage from monolithic integration. In the roof BIPV market, we propose the marginal LCOE to quantify PV technologies in terms of cost performance. CZTS with stainless steel will be able to compete with the counterpart CIGS in marginal LCOE under the assumption that its efficiency can be improved to 15%.

### Author contributions

A. W., N. C., and K. S., X. H. convinced the idea and designed the work. A. W., N. C collected the data and developed the database. N. C. provided the algorithm for the cost model and contributed to the analysis. K. S., C. X., R. E. J. L., C. Y., were involved in discussion and suggestions. The manuscript was written by A. W., N. C., and K. S. All authors contributed to the discussion of the data, writing of the sections of the manuscript and revision of the manuscript.

### Conflicts of interest

There are no conflicts of interest to declare.

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