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An Integrated Assessment of Next Generation PV Technologies

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Abstract: In this study, next generation photovoltaic (PV) materials will be assessed for their viability as the top layer alternatives over crystalline Silicon (c-Si) as the bottom layer in a tandem device architecture. Such a design is critical to ensure effective capture of a broader range of the electromagnetic spectrum, leading to higher value for money and thereby a competitive advantage in the renewable energy market. These evaluations will be conducted through a holistic lens – in understanding not only the science and engineering aspects of a given technology, but through economic viability analyses and considering the ethical, legal, and social implications (ELSI) of it as well. Lastly, with the rapid development of data science – in particular Machine Learning – techniques over the past decade, these new technologies can be smartly modulated to find optimal compositions and fabrication methods that ensure high performance, low cost, and minimal concerns ethically. In the current study, five candidates – CdTe, perovskites, CIGS, CZTS, and a-Si – will be analyzed through these given outlooks and critically gauged against each other to determine their relative strengths and weaknesses. Standard metrics from each outlook domain will be utilized for assessment: from the science and engineering perspective, these will include device stability, degradability, and power conversion efficiency (PCE); price per watt (PPW) and levelized cost of efficiency (LCOE) will be employed for economic viability analyses; acquisition of materials together with toxicity concerns during production and disposal will be probed for ELSI review. It is imperative for the PV industry to adopt this comprehensive approach in its materials' choices and assessments to ensure a mature and sustained growth.

Keywords: Next Generation PVs, Solar, Tandem, Economic Viability, Machine Learning, ELSI

1. Introduction

With the rising demand of feasible alternatives to fossil fuels in the Clean Energy sector, photovoltaics (PV) has become a promising area of focus as they provide high efficiency, low cost of manufacturing, and excellent stability over the course of their lifetimes [1]. Crystalline Silicon (c-Si) is the prevalent absorber layer material in existing solar devices; however, there is a theoretical practical limit of 33% known as the Shockley-Queissar Limit [2]. As the c-Si technology has neared this limit, improvement in performance has stagnated; critically as well, while processing costs have fallen in recent years, that is not enough for this technology to compete with traditional power generation utilizing fossil fuels. In the past two decades, various materials have been investigated as potential alternatives. This current study will focus on a few of such promising materials: Cadmium Telluride (CdTe), Copper Indium Gallium Diselenide (CIGS), Copper Zinc Tin Sulfide (CZTS), amorphous silicon (a-si), and perovskites (a material that follows an ABX_3 structure: "A" being a cation such as methylammonium, "B" being a metal such as lead (Pb), and "X" being a halide, such as Iodine (I)).

As the above technologies have matured and evolved, so has the device architecture of a typical solar device, moving beyond the standard single-junction to tandem, or multijunction, structures. As an example of such a device, focusing on a two-junction format, there are two different regions for light to be absorbed by having a second absorber material overlayed on top of the base material. The appeal of the tandem model is its ability to tap into a larger segment of the electromagnetic spectrum – the top layer with higher bandgap absorbs higher energy photons, with lower energy photons filtering through and being absorbed by the lower bandgap material in the bottom. Figure 1 showcases a perovskite-on-c-Si tandem device, where preferential absorbance of the electromagnetic spectrum by the two absorber materials leads to significant improvement in performance. The low fabrication cost of manufacturing an 'additional' layer in the tandem device compared to the higher gain in device efficiency, or output performance, provides more value for money.

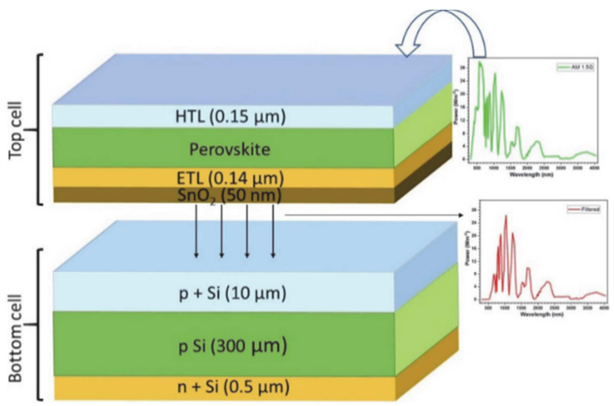

Figure 1. *Schematic representation of the perovskite-on-c-Si tandem device where the top perovskite cell is illuminated under standard solar spectrum and the bottom c-Si cell is illuminated by the filtered spectrum from the top cell.*

When considering the viability of a solar device or module (assembly of connected solar devices making a finalized consumer product), power conversion efficiency (PCE) is one of the key metrics to assess performance in converting sunlight to electricity (ratio of output electrical power to input solar power). Additionally, materials degradability, and stability must be considered as well. Degradability is the propensity of the absorber material to chemically break down under constant irradiation of sunlight. Stability refers to how stable the PV device or module is in producing constant power (by converting sunlight to electricity) under varying environmental conditions such as temperature, humidity, etc. In the current investigation, these three concepts are utilized to determine the overall viability of a solar device from a scientific and engineering basis.

Economic viability must additionally be considered when performing an analysis of different PV technologies. One of the key metrics for the economic viability of a solar technology is the price per watt (PPW). The PPW is a measurement calculated by taking the total cost of the system (usually the solar module) and dividing it by the number of watts of capacity produced by the system when in operation. Additionally, levelized cost of efficiency (LCOE) is a critical metric that can be utilized to assess the feasibility of a given technology from a production cost perspective. This is a metric that measures the overall cost of a PV module over its entire lifetime, typically 25 years [3].

Performing an analysis of each PV technology through an ELSI (ethical, legal, and social implications) lens is the third and final modality considered for the analysis in this current investigation. ELSI can determine if a given technology is feasible when considering various crucial factors such as material acquisition during device/module fabrication (is the material from a conflict region of the world, for example) together with health and environmental considerations (is the material toxic, for example). This is an important metric to consider as certain materials can be inherently toxic for both the environment or public consumption and use as well as during disposal. Other materials may be ethically problematic to acquire – such as tellurium.

In all, each PV technology will be analyzed comprehensively through a suite of scientific and engineering, economic viability, and ELSI based metrics. Such an approach is crucial to ensure that this critical Clean Energy sector evolves in a responsible and sustainable manner. Each PV technology will be assessed and compared against each other, and both qualitative as well as quantitative analytics will be formulated and discussed.

2. Methodology

For the materials considered – amorphous silicon (a-si), Cadmium Telluride (CdTe), Copper Indium Gallium Diselenide (CIGS), Copper Zinc Tin Sulfide (CZTS), and perovskites – each material was analyzed and reviewed on the basis of science and engineering, economic viability, and ELSI. Scholarly review articles and mainstream publications were reviewed, and information was gathered for each of the materials to construct a comprehensive review of each that could be both individually analyzed, as well as compared against each other. Each technology – through these three lenses – were analyzed and assigned various metrics that enabled meaningful comparisons. For science and engineering, device power conversion efficiency (PCE), material stability, and degradability were assessed. For economic viability, material price per watt (PPW), and levelized cost of energy (LCOE) were assessed. Lastly, for ELSI, material acquisition, environmental impacts, and toxicity were assessed. Each of these metrics were considered on a qualitative scale and then translated into a quantitative data set for a basis of comparison. These details are provided under Section 4 – Comparative Assessments of the Various PV Technologies.

3. Results & Discussion

3.1. Cadmium Telluride (CdTe)

3.1.1. Science and Engineering

Cadmium Telluride (CdTe) solar cells are rather impressive from a science and engineering standpoint. The PV market for thin film CdTe solar cells is highly successful and the advancement of CdTe has ramped up considerably over the last decade. CdTe thin film cells perform close to that of conventional c-Si devices. Single junction CdTe cells have achieved a record PCE value of 22.1% while also having a Shockley-Queisser or theoretical maximum of about 32% [4]. In reality, the efficiency of a commercial thin film CdTe solar device is closer to 19.3%, which is in reference to industry data [5]. When it comes to CdTe-on-c-Si tandem solar cells, research is currently underway and theoretical efficiencies have surpassed single junction CdTe limits with a 38% theoretical tandem PCE [6]. However, a significant obstacle for CdTe-on-c-Si tandem solar cells is the fact that the electronic bandgap of both materials are closer than ideal (ideally, the top and bottom materials should have significantly different bandgaps to effectively tap into distinct parts of the electromagnetic spectrum). As a result, alloying Zinc (Zn) and Magnesium (Mg) with CdTe increases the compatibility and allows for a successful tandem device. This alloying addition, however, unfortunately reduces the efficiency of the CdTe absorber layer, yielding a less efficient tandem cell compared to that of a single junction CdTe cell. In fact, CdZnTe and CdMgTe cells only achieve efficiencies of 16.4% and 11.2% respectively [1]. Nonetheless, CdTe-on-c-Si tandem solar cells are still a possible candidate for commercial applications as companies such as FirstSolar and SunPower are exploring these technologies in order to achieve greater efficiency than that of single junction CdTe cells. Also, because of the inorganic nature of CdTe, it has an advantage of considerably better stability compared to their organic counterparts. This is not unique to just CdTe, but rather the case for most inorganic PV cells. Lastly from a degradability perspective, CdTe PV cells have similar statistical degradation rates to that of standard c-Si. CdTe and c-Si differ in when degradation happens in their life cycles. CdTe will begin to rapidly degrade initially and then flatten out over time, whereas c-Si PV cells tend to degrade much later in their life cycles [1]. This opposition in degradability between the two promotes promising results for next generation CdTe-on-c-Si tandem cells, which is an area of focus in FirstSolar's next generation solar panels. Due to the popularity of CdTe solar cells, some innovative engineering is taking place in the market. Companies such as Antec Solar, Solar Scape Enterprises, A-Grade Energy, Advanced Solar Power, Lucintech, Optimum Sun, Polysolar, RK Solar, and Solar Motion have developed CdTe Building-Integrated PV (BIPV). BIPV either works in conjunction with, or takes the place of, traditional glass windows, sunroofs, skylights, external masonry, and any other building materials. The optical and thermal performances of CdTe have been found to be superior compared to the rest of the materials in this study, leading to its application in the BIPV markets [3]. These types of applications will undoubtedly increase the usage and relevance of the solar industry as a whole.

3.1.2. Economic Viability

CdTe solar cells are fairly competitive with industry standard c-Si technology from an economic viability standpoint as well. CdTe is a current production technology with vast markets globally. It is known that it is the second most sold PV technology globally, coming in just behind c-Si. Manufacturers from the USA, Germany, and China supply a majority of the global markets on CdTe. Companies such as First Solar, Toledo Solar, Antec Solar, CTF Solar, Lucintech, RK Solar, Solar Motion, and Solar Scape Enterprises are thriving primarily from CdTe sales. This is plausible as CdTe modules are estimated to cost $.28/Watt in a 2020 statistic – a competitive value compared to the traditional c-Si technology. By 2030, CdTe module cost is estimated to be as low as $.18/Watt putting them at par with bifacial c-Si PV technology [7]. However, this is not the best PPW estimated for 2030, that is held by CIGS at $.10/Watt (to be discussed below). The LCOE of CdTe in 2020 was $0.05/kWh and is projected to fall to $0.03/kWh by 2030 [7]. The competitive cost of CdTe is directly proportional to the good efficiency, stability, and degradability of the technology, as well as the industry and academia R&D that surrounds the technology and its advancements.

3.1.3. ELSI

The setbacks and limitations of CdTe PV technology are undoubtedly in its ethical, legal, and social Implications (ELSI). It is known that Cadmium (Cd) is a highly toxic material both to nature as well as to humans. Although it is a naturally occurring element within the earth, concentrations are considerably low as Cd is not found as a pure element, but rather as a mineral combined with oxygen, chlorine, or sulfur [8]. Almost all of the world's acquisition of Cd is from China as a byproduct of Zinc mining. Although China has made legal reforms to the monitoring and control of pollution from industry, it is a focused effort towards smog air particulates in general. As of now China has little to no legal implications when it comes to the care and handling of Cd specifically, or oversight of Cd pollution from mines and smelters, and environmental contamination of Cd. Studies show that Cd soil and water contamination near Zinc mines and Copper smelters has an alarming impact on crops, livestock, and population within the vicinity [9]. However, there are current Chinese proposals and possible future reforms in the making to address this ethical issue of Cd contamination. This oversight falls under China’s Ministry of Ecology which, by 2025, aims to implement and enforce strict regulations of heavy metal pollution, create standard measures, promote a clean product transformation, invoke a permit system for regulated pollution, and control location placement of applicable companies [10].

When it comes to Tellurium (Te), it is considerably less toxic than that of Cd. However, the CDC recommends proper respirators dependent on measures of Time Weighted Average (TWA) air sampling [11].

Acquisition and handling of raw materials for CdTe is by far the most problematic issue of the technology. Once formed into CdTe the toxicity is greatly reduced by approximately two to three orders of magnitude compared to that of Cd alone. CdTe also has vast differences in chemical and physical properties compared to that of either Cd or Te. For instance, sources [12] point out that the melting point of CdTe is 1041°C, compared to that of 321°C and 449°C, for Cd and Te, respectively. It is CdTe's properties and relatively low toxicity that contribute directly to a good standing Life Cycle Assessment (LCA). LCA studies determined that in the worst case scenario where 100% of the semiconductor is released into the environment due to rainwater, the potential Cd concentrations are below heath screening levels for Soil, Air, and Groundwater [12]. These studies also show that the recyclability of CdTe PVs has a considerably lower environmental impact than that of Si PVs. These studies were carried out according to recycling procedures that were already commercially implemented. The metrics of comparison included recycling and energy recovery of materials as well as further treatment and disposal of solid and liquid wastes. Although values fluctuated from recycling process variations, these results were comparatively better for CdTe over Si. [12]

When it comes to manufacturing, there are regulations and legal implications for most countries involved. For instance, American companies such as FirstSolar and Toledo Solar are regulated by agencies such as Occupational Safety and Health Administration (OSHA) and Environmental Protection Agency (EPA) and many more. Apart from external regulations, a case study of FirstSolar has revealed that production quality and safety are top priorities. Precautions such as air quality monitoring, employee biomonitoring, standardized production processes, intensive employee training, and random product batch reliability testing are just some of the measures done to ensure the safety of employees, surrounding communities, and the environment [12].

3.2. Perovskite

3.2.1. Science and Engineering

The inception of perovskite materials was through the naturally occurring mineral of Calcium Titanate ($CaTiO_3$), discovered in 1839 by the German mineralogist Gustav Rose and named after Russian mineralogist Lev Perovski. Ensuing materials with the same crystal structure are also considered as perovskites, consisting of a general formula, ABX_3. Here, "A" are organic cations, "B" are metal cations, and "X" are halide anions. There are two variations of perovskites – halide and non-halides – that are used as the absorber material in the PV technology (Solar Energy Technologies Office, Department of Energy, n.d). Perovskite solar device PCE numbers almost parallel those of c-Si and this technology is a great low cost alternative in the PV industry. Perovskite solar devices have undergone a meteoric rise in PCE, from 3% in 2009 to over 25% currently, making it likely the most promising PV technology yet. In spite of great promise, there are quite a few obstacles for perovskites to become a sustainable commercial technology. The durability of the light absorbing perovskite material is one of its greatest obstacles, as it can decompose when reacting to natural elements such as moisture and oxygen as well as when exposed to light, heat, or applied voltage for extended periods of time [13]. As global research is pivoted in tackling these challenges, perovskite-on-c-Si tandem devices are an extremely promising Next Generation technology which could potentially produce PCE values of over 33%. Critical properties of these materials such as their absorption range can be chemically tuned easily, leading to versatility in complementing a bottom layer in the tandem architecture to.

3.2.2. Economic Viability

One of the key advantages of the perovskite technology is the material's low cost and ease of processability: a typical device contains a thin perovskite absorber layer, which is ~0.3mm thick. Additionally, the layer can be processed through batch-processing and roll-to-roll processing techniques, leading to low production costs overall. The perovskite technology currently requires a PPW of \$0.38/Watt, with further imminent technological advancements looking to halve that number by 2030 [7]. When compared to typical fossil fuel costs of \$0.05-0.07/Watt, perovskites have come a long way to be a competitive alternative energy source. From an LCOE perspective, perovskites boast a rapid reduction from \$4.00/kWh in 2020 to a projected \$0.03/kWh in 2030 [7].

3.2.3. ELSI

While perovskites are an attractive option for the PV industry, certain components in the structure are toxic. The most common material used as the A cation is lead (Pb) as it provides good device performance; nonetheless, Pb creates obvious concerns in terms of health risks and environmental pollution, especially during disposal. During disposal, Pb can leak into the environment including water, creating a quick means of transmission and ingestion [14]. Human impacts include anemia, kidney damage, hypertension, neurological disorder, and cancer. Pregnant women are especially more prone to these effects, and they can result in birth defects and issues with the infant's development. Lastly, the halide of choice – Iodine (I) – can be problematic as well. While Iodine is typically chosen for its high device performance, it too – like Pb – can cause soil and environmental pollution. Its negative impact on plants and ecology can be profound.

3.3. Copper Zinc Tin Sulfide (CZTS)

3.3.1. Science and Engineering

Studies have been conducted investigating the performance of copper zinc tin sulfide (CZTS) based PV devices with different layer configurations. The highest PCE reported for the CZTS based PV devices without a back surface field (BSF) layer was 8.55%. The addition of a CZTSe BSF layer to the FTO/ZnO/CdS/CZTS/CZTSe/Mo configuration has been shown to boost the overall PCE to 22.03% [15]. To date, the best performing structure, FTO/ZnO/CdS/CZTS/CZTSe/Pt, has shown a PCE of 29.86%. Currently two types of thin-film technologies are being investigated, an all in-line vacuum process and a wet process based on colloidal ink spraying [16]. The latter has shown a better device performance than the former. Moreover, long stability tests on wet-processed kesterite devices both under continuous indoor irradiance and in outdoor field tests showed zero or only minor initial efficiency loss. Long accelerated heat tests on monograin-based kesterite devices did not show any significant degradation for certain CZTS compositions. In all, from a science and engineering perspective, CZTS PVs are an exciting and promising option in the current industry.

3.3.2. Economic Viability

CZTS is made from abundant and low-cost materials, making it a cost-effective option for solar devices. CZTS can be used in three different processes: on glass, stainless steel, and plastic, with estimated costs of less than $.50/Watt for each [17]. Crystalzol reported a PPW cost of $.35/Watt for CZTS on plastic.

3.3.3. ELSI

Like any emerging technology, there should be ethical, legal, and social implications associated with CZTS and its constituent elements. The mining and extraction of copper, zinc, tin, and sulfur can have significant environmental impacts. Copper mining, for example, often involves the use of large quantities of water and energy and can result in the release of toxic byproducts such as sulfuric acid and heavy metals. Zinc mining can also have similar impacts, and the extraction of tin can contribute to deforestation and habitat destruction [18]. The production of CZTS solar devices requires the synthesis of the CZTS material, which involves the use of high-temperature processes and toxic chemicals [19]. While researchers are working to develop more sustainable and less hazardous methods for CZTS synthesis, it remains an area of concern for the ethical and social implications of CZTS technology.

3.4. Copper Indium Gallium Diselenide (CIGS)

3.4.1. Science and Engineering

CIGS is an inorganic PV technology which has a competitive market in the portable electronics industry as well as for small off grid solar panels for RVs. An advantage of the CIGS devices is the flexibility compared to the conventional c-Si PV device. Currently, the CIGS technology makes up about 2% of the current market share of PV technology shipments. The technology has been reportedly worked on since the 1970s by Showa Shell (Solar Frontier) but has only recently been studied in depth during 2010 and onward. CIGS solar devices were first synthesized in 1953 by Harry Hahn [20]. These devices have a lifespan of around 25 years with PCE numbers fairly invariant under temperature fluctuations [21]. This is due to the low temperature coefficient of the material. Average PCE numbers range in the 12-14% range for a module [22]. The current highest reported CIGS device PCE exceeds 24% and has grown quickly; the highest reported PCE in 2005 was just 15%. CIGS modules are mainly manufactured in Japan by the company Solar Frontier.

3.4.2. Economic Viability

CIGS, in bulk, cost $400-$450/kg [23]. For the PPW metric, CIGS solar cells produce $.48/Watt (Solar Frontier, n.d) with a projection to drop to $0.10/Watt by 2030. The LCOE of CIGS in 2020 was $0.06/kWh and is projected to drop to $0.03/kWh in 2030 [7].

3.4.3. ELSI

In terms of carbon footprint, CIGS PV technology has a very clear advantage over c-Si. While commoditized mono c-Si has a carbon footprint of 50–60 g CO_2 equivalent/kilowatt hour of electricity, the carbon footprint of thin film CIGS is only 12–20 g CO_2 equivalent/kilowatt hour [24]. The concerns for Cadmium and Selenium are similar to those for CdTe as described previously.

3.5. Amorphous Silicon (a-si)

3.5.1. Science and Engineering

Amorphous Silicon (a-si) at the onset can appear as a promising PV candidate due to its low cost in manufacturing and consistent PCE output. However, the PCE values typically realized by a-Si as single junction devices are low when compared to alternative cells in the PV sector. a-Si is a non-crystalline form of silicon that typically provides a PCE of 7-8% and a record conversion efficiency of 10.2% [1]. Therefore, from a scientific viability standpoint, this is a low value; additionally, not much progress has been made in the development of single junction a-Si devices. One of the downsides of a-Si is that it suffers from high degradability and low stability over the course of its lifetime. a-Si PV devices experience a lifetime of roughly 2-3 years which is significantly less when compared to its c-Si counterpart (WSL Solar). This performance degradation that the material suffers upon light soaking has been investigated well, and is known as the Staebler Wronski effect [25]. This effect causes a light induced creation of defects in the absorber layer, leading to obvious impediments in implementation in the commercial sphere.

3.5.2. Economic Viability

a-Si is a promising candidate from an economic viability front due to its low cost of manufacturing when compared to the traditional c-Si modules. An established history in manufacturing and low material costs make it a suitable candidate for large scale applications [26]. As mentioned previously, while a-Si is appealing from an economic standpoint when compared to c-Si, this technology is considerably weak from a PCE standpoint. a-Si is more promising in the area of low power electronics, rather than large scale consumer or industrial solar farms. Through data collection and analysis, there were no reliable standard LCOE or PPW figures reported, lending to the idea that this particular absorber layer is not feasible in the next generation photovoltaic assessment.

3.5.3. ELSI

Similar to crystalline silicon (c-Si) there are no crucial ethical concerns to note for a-Si. This material is relatively safe for use in PV devices.

3.6. Crystalline Silicon (c-Si)

3.6.1. Science and Engineering

Crystalline Silicon is the absorber layer used for comparison in this analysis as it is the most established and widely used material to date due to its high PCE as a single junction absorber layer, as well as its high stability and low degradability. In a commercial setting, c-Si modules showcase a consistent PCE of 18-20% [27], while on the cell level, these devices can range from 20-25% for multi crystal and single crystal cells. The need for next generation photovoltaic cells however comes from the fact that c-Si solar cells have low opportunity for growth, having crept up over the past decades towards its maximum theoretical conversion efficiency known as the Shockley-Quessier limit, which as previously mentioned, is 33%. There are of course losses which lower the PCE from this theoretical limit. These high PCE numbers, however, have not been able to offset the still high processing costs, making this quintessential technology not competitive with fossil fuels. There is therefore an imperative for the photovoltaic industry to grow through the advancement of tandem and next generation photovoltaic devices. c-Si does yield a high stability with an average module lifetime of 20-25 years [28]. As a result of this long lifetime, it is clear additionally that these cells fare well against ambient conditions and do not have a high degradability.

3.6.2. Economic Viability

Currently, c-Si constitutes the highest global import of all photovoltaic modules with 95% being monocrystalline Silicon. [29]. c-Si requires an average Price per Watt of $0.20/W to $0.40/W [30]. These prices are known to fluctuate however, with a focus on lowering the overall kWh of the modules to increase demand in the market. Current LCOE of the best performing c-Si technologies is between $0.03-$0.06/kWh [31].

3.6.3. ELSI

Overall, Silicon is one of the most abundant elements found within the earth's crust and c-Si devices and modules when compared to other absorber layer devices, do not present any serious harm to either the environment or to those populating it. They have a consistently large lifespan and overall are one of the safer devices. Current research and technology are seeking to maintain this standard of consumer safety while attempting to improve the scientific/engineering and economics metrics.

4. Comparative Assessments of the Various PV Technologies

As previously discussed, each of the five technologies were analyzed through each relevant category of science and engineering, economic viability, and ELSI.

4.1. Science and Engineering

Utilizing discussions in the previous section as qualitative data, each of the five technologies were ranked against each other based on their PCE, degradability, and stability. The results of these analyses are depicted in Figure 2.

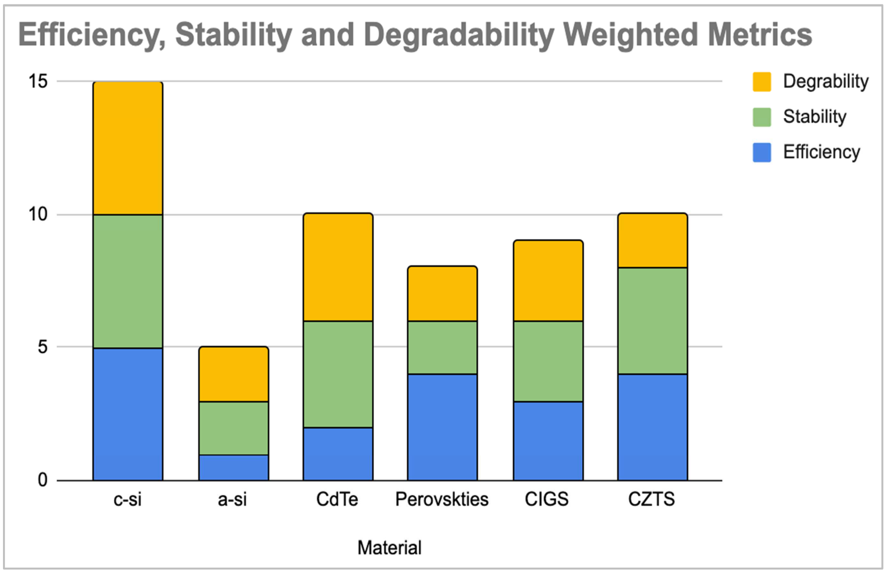

Figure 2. *Efficiency, Stability, and Degradability Metrics.*

For these analyses, each of the given technologies were ranked in the three categories on a scale of 1 to 5, with 1 being the least ideal, and 5 being the most promising. As mentioned in the Methodology section, each of the five technologies were compared to c-Si, which has been the standard absorber layer in the PV industry. For the sake of these measurements, c-Si was assigned a score of 5 across all metrics as it is at this time the most reliable to reach a consistent PCE, has favorable stability and has minimal degradation over time. Figure 1 showcases how converting qualitative data into its quantitative counterpart utilizing the three highlighted metrics provides a clear picture of the strengths and weaknesses of each PV technology when compared to not only c-Si, but against one another.

4.2. Economic Viability

Just like in Section 4.1.1, the metric employed for PPW (price per watt) was measured on a comprehensive scale ranging from 1 to 5, with each ranking based over a range of 10 cents. For instance, the range of $0 – $0.1/Watt corresponded to a ranking of 5, while $0.11 – $0.2/Watt represented a ranking of 4, and so on. The higher the rankings, the better a given material's performance. This approach facilitated a linear assessment of PPW values, enabling direct comparisons. LCOE was similarly assigned a ranking of 1 through 5 for the given technologies. The PPW and LCOE data that was available was translated into Figure 3.

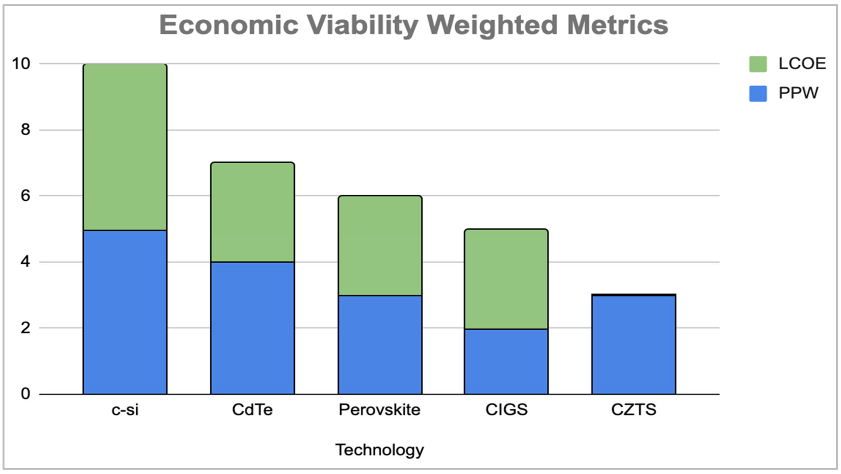

Figure 3. *PPW and LCOE Metrics.*

Figure 3 reveals that, when viewed from an economic perspective, after c-Si, CdTe emerges as the most cost-effective absorber layer among the analyzed materials. Unfortunately, reliable data for a-Si, which was previously discussed, could not be obtained, and thus was not taken into account. Similarly, LCOE data for CZTS was unavailable and not considered. Nevertheless, a comparison of CdTe, perovskite, and CIGS demonstrates that CdTe stands out as the most economically advantageous option.

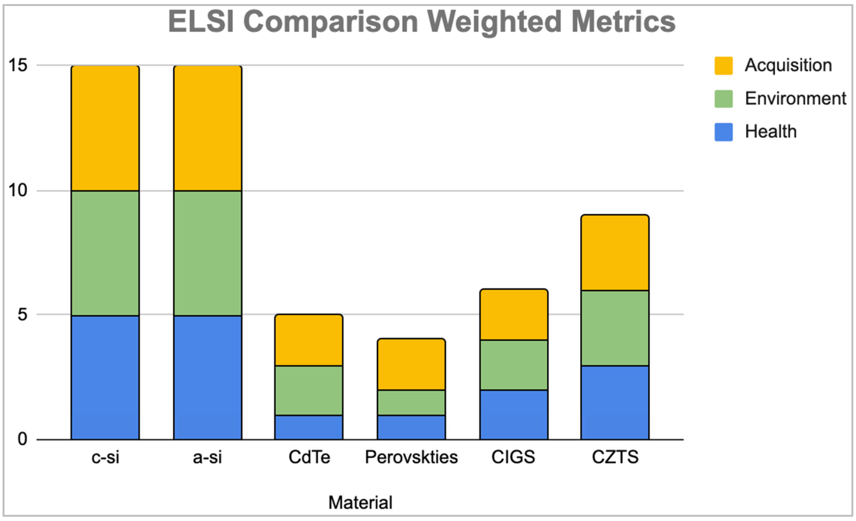

Figure 4. *ELSI Metrics.*

4.3. ELSI

Using a similar approach to Sections 4.1.1 and 4.1.2, the ELSI of each technology was compared against one another on a numerical scale of 1 to 5. As before, 5 is the most ideal ranking, and 1 is the least. The results are shown in Figure 4.

In this case, the metrics analyzed were materials acquisition, environmental impact, and concerns to health and public safety. As can be seen, a-Si and c-Si showcase the most favorable choices from the ELSI perspective, with the largest bars. It can additionally be observed that while CdTe, CIGS and perovskites are expected to be favorable from a scientific/engineering or even economic viability perspective, their ELSI impacts are concerning. It can also be observed that CZTS fares better in ELSI than these three technologies.

5. Machine Learning / AI / Accelerated Discovery

While each of the materials investigated in this study are promising in their own right when considered as next generation PV technologies (defined previously as a tandem architecture utilizing each material as a top layer option over c-Si as bottom layer), Machine Learning (ML) approaches can be considered to greatly accelerate the rate at which suitable material compositions are discovered. Powerful computational techniques such as density functional theory (DFT) utilized to probe materials properties, in conjunction with realistic device simulation tools such as WxAMPS or SCAPS, can be used to investigate the PCE of a particular solar device prior to lab based fabrication. Savvy ML models can add a further layer of clarity in showcasing ideal materials composition as well as fabrication techniques to make devices that are commercially feasible from the perspective of the three criteria highlighted in this study – science/engineering, economic viability, and ELSI. Perovskites are an excellent example of a technology that can be probed through ML models to satisfy these criteria. ML models can be used to find substitutes for lead (such as tin or bismuth) and iodine (such as bromine). [32]. Improving on the ELSI front will complement the science and engineering aspect of the technology, thereby increasing its viability in the clean energy market. Additional examples of materials that may be suitable for alternative compositions include CdTe, which requires alternatives to replace the toxic material Cadmium and the rare material Tellurium obtained from conflict regions. With favorable scores already in the science/engineering and economic feasibility spheres, an improvement in the ELSI metric can catapult this technology to being a stable and sustainable contender in the PV market. This approach of utilizing ML models can be considered for any of the absorber layer materials discussed, and innumerable device data can be analyzed in a relatively short period of time utilizing ML models, thus greatly accelerating the findings and discovery for ideal compositions and fabrication methods for a given technology.

6. Conclusion

With a global pressure placed on the Clean Energy sector to find viable and sustainable alternatives to fossil fuels, PV technologies are an extremely promising candidate due to their low cost of manufacturing and promising efficiencies. The standard absorber material in the PV world has been crystalline silicon (c-Si) for many decades; however next generation tandem device architectures, where new materials are fabricated on top of a base c-Si layer, can be promising in terms of exceeding the Shockley-Queisser limit of 33% PCE while providing lower PPW and LCOE (offering more value for money). In the current study, five candidates – CdTe, perovskites, CIGS, CZTS, and a-Si – were analyzed through the lenses of science and engineering, economic viability, and ELSI to determine the strengths and weaknesses of each of these technologies. While some materials may be relatively promising from a scientific perspective, they may raise concerns from an economic viability or ELSI perspective, and vice versa. With the methods utilized herein, the current study reports tied highest rankings of CZTS and CdTe in the science and technology space, highest ranking of CdTe in the economic viability arena, and highest ranking of CZTS after a-Si in the ELSI realm. The tremendous impact and scope of accelerated discovery through ML models have also been highlighted. It is imperative to assess each PV technology with the holistic view proposed herewith in order to make decisions moving forward in realizing a mature and sustained PV industry.

Data Availability Statement

Any data will be made available on request.

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