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Article

Material and Device Parameter Optimization for High-Efficiency Silicon, CdTe, CIGS, and Perovskite Solar Cells: A Comparative SCAPS-1D Simulation Study

Vijay Aithekar[1*], Dr. Amit Saxena[2]

[1*,2]Department of Science, Oriental University, Indore (M.P.)
[1*]Correspondence author Mail Id: vijayaithekar@orientaluniversity.in

Abstract: The simulation results provide a clear comparison of how the bandgap and material properties of different absorber layers influence the performance of solar cells. The analysis shows that the bandgap of an absorber plays a major role in determining the balance between the generated current and the achievable voltage. Materials with bandgaps in the range of about 1.3–1.5 eV are particularly attractive because they can make effective use of the incident solar spectrum while maintaining a relatively high output voltage. When recombination losses are kept low, such materials have the potential to deliver efficiencies close to the theoretical Shockley–Queisser limit. On the other hand, a large voltage deficit generally indicates significant recombination losses, which reduces the practical efficiency of the device. The thickness-dependent simulation of the perovskite absorber shows that the device achieves its best performance at an absorber thickness of approximately 400–500 nm, with a maximum power conversion efficiency of around 21%. Increasing the thickness beyond this range does not necessarily lead to a corresponding increase in efficiency, as additional material can also increase carrier recombination. Similarly, using an excessively thin absorber may reduce light absorption and consequently limit the short-circuit current density. Therefore, selecting an appropriate absorber thickness is important for obtaining a suitable balance between optical absorption and electrical losses. The influence of defect density is also significant. The simulation indicates that reducing the bulk defect concentration to below 1×10^{15} cm^{-3} produces a noticeable improvement in both the open-circuit voltage (VOC) and fill factor (FF). A lower concentration of defects reduces the number of recombination centers within the absorber, allowing a greater proportion of the photogenerated charge carriers to contribute to useful current. This highlights the importance of controlling material quality during the fabrication of high-performance photovoltaic devices. The bandgap comparison further indicates that absorbers with bandgaps close to approximately 1.34 eV, including CdTe and suitably designed perovskite materials, can achieve relatively high simulated efficiencies. Their favorable bandgap and lower recombination losses provide a better balance between voltage generation and current production. In comparison, materials suffering from larger voltage losses show a greater departure from their theoretical efficiency potential. An important outcome of the study is that perovskite absorbers can achieve high efficiency using comparatively thin active layers. This feature can reduce material requirements and supports the development of lightweight and potentially low-cost photovoltaic devices. Overall, the results demonstrate that careful control of bandgap, absorber thickness, and defect density is essential for improving solar-cell performance. The findings also provide useful guidance for future device optimization and the development of efficient photovoltaic technologies for sustainable energy generation.

Keywords: Perovskite solar cells; Bandgap engineering; Absorber thickness; Defect density; non-radiative recombination; Open-circuit voltage; Fill factor; Power conversion efficiency; Shockley–Queisser limit; Photovoltaic performance; Solar-cell optimization; Thin-film photovoltaics

1. INTRODUCTION

1.1 Silicon and Thin-Film Baseline

Solar photovoltaic (PV) technology is one of the key options for meeting the growing demand for clean and sustainable energy. Continuous developments in absorber materials, device structures, and fabrication techniques have resulted in steady improvements in solar-cell performance [1]. Among the commercially established technologies, crystalline silicon (c-Si) continues to dominate the photovoltaic market because of its high efficiency, good reliability, and proven long-term stability [2]. Advanced conventional c-Si solar cells have achieved laboratory efficiencies of approximately 26–27%. However, silicon has an indirect bandgap of about 1.12 eV, resulting in relatively weak light absorption. Consequently, effective absorption of sunlight requires high-purity silicon wafers with typical thicknesses of around 150–180 μm. The use of thick wafers increases material consumption and can add to the overall manufacturing cost [3].

Thin-film technologies, particularly cadmium telluride (CdTe) and copper indium gallium selenide (CIGS), offer an attractive alternative because their absorber layers can be considerably thinner than those used in silicon devices. Both technologies have achieved power conversion efficiencies exceeding 20%, with CdTe and CIGS cells reporting efficiencies of about 22% and 23%, respectively [4]. Despite these achievements, their performance is still influenced by material and interface-related losses. Defects associated with grain boundaries and imperfections within the absorber can increase carrier recombination, thereby reducing the voltage and current collected from the device. Furthermore, unsuitable energy-band alignment between the absorber and adjacent transport layers can hinder efficient carrier extraction and adversely affect the open-circuit voltage and fill factor [5]. Therefore, controlling defect-related losses and optimizing the electronic properties of interfaces remain important strategies for further improving the performance of thin-film photovoltaic devices.

1.2 Perovskite Emergence

Metal-halide perovskite solar cells (PSCs) have emerged as one of the most promising photovoltaic technologies of the past decade [6]. Their rapid development is mainly associated with the favorable optical and electronic properties of perovskite absorber materials, commonly represented by the ABX_3 crystal structure. Since the first notable demonstrations, the reported efficiency of perovskite devices has increased dramatically, from about 3.8% in 2009 to more than 25% in single-junction cells [7]. This rapid progress has placed perovskites among the leading candidates for next-generation photovoltaic applications. Single-junction perovskite devices have achieved efficiencies comparable to those of established silicon technologies, with certified efficiencies of approximately 25.7% and open-circuit voltages (VOC) approaching 1.1 V [8].

One important advantage of perovskite materials is their ability to tolerate a considerable concentration of intrinsic defects without causing severe performance degradation. Many defects form shallow electronic states rather than deep recombination centers, which helps suppress non-radiative recombination and supports high VOC values [9]. In addition, typical perovskite compositions possess bandgaps in the range of about 1.5–1.6 eV, which is favorable for efficient single-junction solar-energy conversion. The theoretical efficiency of such devices can approach 30%, while the Shockley–Queisser limit is around 33% for an ideal bandgap near 1.34 eV [10].

Another major benefit is the strong absorption coefficient of perovskite materials. More than 90% of visible sunlight can be absorbed within a layer only a few hundred nanometers thick, considerably reducing the amount of absorber material required compared with crystalline silicon [11]. This feature makes PSCs attractive for lightweight and potentially low-cost photovoltaic applications. Nevertheless, long-term stability under moisture, heat, oxygen, and illumination remains a major concern. Further progress will therefore depend on improving material stability, reducing defects, and optimizing interfaces and device architecture.

1.3 Motivation for Simulation Study

Despite the rapid progress of photovoltaic technologies, the key factors controlling voltage, current generation, and fill factor are not always clear across different absorber materials. Experimental optimization can require considerable time and resources, making numerical device modelling a useful alternative for studying individual

material and device parameters. In this context, SCAPS-1D provides a practical platform for examining the effects of absorber thickness, defect density, doping concentration, bandgap, and interface properties on solar-cell performance.

A comparative study of silicon, CdTe, CIGS, and perovskite solar cells can therefore provide a better understanding of the factors responsible for their different efficiencies. By varying selected parameters independently, device-level simulations can identify their influence on important photovoltaic characteristics such as VOC, JSC, FF, and PCE. The present analysis focuses particularly on understanding why perovskite cells can achieve high voltage with very thin absorber layers, identifying possible routes for further improvement, and comparing their performance with established photovoltaic technologies.

2. Literature Review

2.1 Silicon Solar Cells – Baseline Technology

Crystalline silicon (c-Si) has been the leading photovoltaic material for several decades and continues to serve as an important benchmark for evaluating emerging solar-cell technologies. Its success is mainly due to its reliable performance, excellent stability, and well-established manufacturing infrastructure. Advanced single-junction silicon cells have achieved laboratory efficiencies in the range of 26–27%, showing that the technology is already highly optimized [12]. Silicon has an indirect bandgap of approximately 1.12 eV. Although this bandgap allows the material to utilize a broad portion of the solar spectrum, its relatively weak absorption means that conventional devices require comparatively thick wafers, generally about 150–200 μm, along with suitable light-management structures to improve photon absorption [13].

High-quality silicon contains relatively few electrically active defects, allowing photogenerated carriers to travel over long distances before recombination. This contributes to strong current generation, particularly when thick absorbers are used. However, the achievable open-circuit voltage is restricted by the relatively small bandgap and carrier-recombination processes, including Auger recombination. Commercial crystalline-silicon modules have already reached efficiencies above 20%, while improvements in surface passivation and selective contacts continue to reduce electrical losses [14,15].

Device concepts such as PERC and silicon heterojunction cells have further enhanced performance by improving carrier collection and reducing recombination at surfaces and contacts [16]. Despite these advances, silicon manufacturing still involves energy-intensive processing and wafer fabrication, and the rigid structure of conventional wafers limits their suitability for some lightweight applications [17]. Since single-junction silicon cells are now close to their practical efficiency ceiling, future major gains are more likely to come from tandem configurations that combine silicon with another absorber capable of harvesting complementary portions of sunlight.

2.2 Thin-Film Chalcogenide Cells (CdTe and CIGS)

Second-generation photovoltaic technologies such as cadmium telluride (CdTe) and copper indium gallium selenide (CIGS) were developed to overcome some of the material and manufacturing limitations associated with conventional crystalline-silicon cells. Their main advantage is the use of very thin absorber layers, which reduces material consumption while allowing deposition over large areas and, in some cases, flexible substrates. CdTe is particularly attractive because it has a direct bandgap of about 1.45 eV and a very high optical absorption coefficient, typically exceeding 10^5 cm^{-1} [18]. As a result, most useful sunlight can be absorbed within a layer only a few micrometers thick. CdTe devices generally employ absorber thicknesses of around 2–4 μm, and increasing the thickness beyond this range provides only a limited improvement in photocurrent [19].

Modern CdTe cells commonly used CdS or related window layers together with carefully engineered rear contacts. High-performance devices based on CdSeTe alloys have demonstrated efficiencies above 22%, with current densities close to 30 mA/cm², open-circuit voltages near 0.88 V, and fill factors approaching 80% [20]. However, the voltage remains significantly below the theoretical value expected from the CdTe bandgap. This difference is associated with recombination losses arising from defects, grain boundaries, interfaces, and imperfect rear-contact

properties. Consequently, defect passivation and back-contact engineering remain important routes for improving CdTe performance [21, 22]. Commercial CdTe modules have also demonstrated good outdoor performance, particularly under elevated operating temperatures, while maintaining the cost advantages of thin-film manufacturing [23].

CIGS is another important thin-film technology with a direct bandgap that can be adjusted by changing its elemental composition [24]. Its strong absorption allows efficient operation with absorber layers of roughly 1–2 μm. Laboratory CIGS-based devices have achieved efficiencies above 23%, demonstrating the potential of bandgap control, alkali-metal treatments, and improved buffer layers for reducing recombination losses [25–27]. The open-circuit voltage of conventional CIGS devices is generally lower than the bandgap would suggest, indicating that defects and interface recombination remain important limitations. Treatments involving elements such as sodium and potassium have been found to improve carrier collection and reduce recombination losses [28].

Both CdTe and CIGS offer significant advantages in terms of thin absorber layers, scalable manufacturing, and established commercial applications. However, the availability and cost of some constituent elements, particularly tellurium, indium, and gallium, remain considerations for large-scale deployment.

For CdTe and CIGS, further efficiency gains depend mainly on reducing voltage losses caused by recombination, grain-boundary defects, and unfavorable interface band alignment rather than improving light absorption.

2.3 Perovskite Solar Cells

Halide perovskite solar cells have developed remarkably quickly and have become an important area of research in photovoltaic technology. The first perovskite-based solar cell was reported by Kojima and co-workers in 2009, with an efficiency of about 3.8% [29]. Since then, considerable progress has been achieved through improvements in chemical composition, surface and interface treatment, charge-transport layers, and overall device structure. These developments have raised the efficiency of perovskite solar cells to around 25% in certified laboratory devices [30].

Perovskite materials, including methylammonium- and formamidinium-based lead halides, offer adjustable bandgaps that can generally be tuned within the range of about 1.5–1.7 eV. Their strong absorption and sharp absorption edge allow efficient harvesting of sunlight using very thin absorber layers. With absorption coefficients of approximately 10^5 cm^{-1}, a perovskite film only a few hundred nanometers thick can absorb a large fraction of the incident visible radiation [31]. The small absorber thickness, together with solution-based deposition methods, creates opportunities for lightweight, flexible, and potentially low-cost photovoltaic modules [32].

Another notable feature of perovskites is their relatively high open-circuit voltage. High-quality devices can produce VOC values of approximately 1.15–1.20 V for bandgaps around 1.5–1.6 eV, indicating comparatively small voltage losses. This behavior is closely related to the low density of electrically active defects and reduced non-radiative recombination. Good-quality perovskite films can exhibit defect concentrations near or below 10^{15} cm^{-3}, while carrier diffusion lengths can extend over several micrometers [33].

Device architecture also strongly influences performance. Low-temperature electron-transport layers such as SnO_2 can help reduce interface-related losses [35]. Inverted p–i–n structures using materials such as NiO or PEDOT:PSS as hole-transport layers, together with fullerene-based electron-transport layers, have also shown improvements in hysteresis behavior and device stability [36].

3. Simulation Methodology

Each device was modeled in a standard p–i–n or n–i–p configuration, depending on the technology. The typical layer stacks used are summarized below:

- Perovskite cell: glass/ITO (front contact) / compact TiO_2 (ETL, ~50 nm) / $CH_3NH_3PbI_3$ absorber (nominally intrinsic, ~0.2–1.0 μm) / Spiro-OMeTAD (HTL, ~200 nm, p-type 10^{18} cm^{-3}) / Au (back contact).

- Silicon cell: standard p–n homojunction with p-type base (10^{16} cm^{-3}, 180 µm) and n-type emitter (10^{18} cm^{-3}) corresponding to wafer-based devices.
- CdTe cell: glass/ITO / CdS window (n-type, 50 nm) / CdTe absorber (p-type, ~3 µm, 10^{14} cm^{-3}) / metal back contact.
- CIGS cell: glass/Mo (back contact) / CIGS absorber (p-type, 2 µm, 10^{15} cm^{-3}) / CdS buffer (50 nm) / ZnO:Al (front contact).

Interface band offsets were introduced as reported in literature—approximately 0.3 eV at CdS/CdTe and CdS/CIGS junctions—to reproduce realistic heterojunction alignments [48][49]. Series resistance (R_s) and shunt resistance (Rsh) values were tuned to yield fill factors (~80%) consistent with champion devices. For instance, the perovskite cell used $R_s \approx 0.3\ \Omega\cdot cm^2$ and $Rsh \approx 10^6\ \Omega\cdot cm^2$.

The intrinsic defect density in absorbers was set to 10^{15}–10^{16} cm^{-3}, varied systematically to study its influence on VOC and FF. Uniform optical generation was assumed through each absorber to focus on electrical transport effects. Baseline models were first calibrated to reproduce characteristic experimental performance metrics for each technology (Table 1), after which parametric sweeps were carried out for:

1. Absorber thickness (especially 0.1–1.0 µm range for perovskite).
2. Defect density (Nt) in the absorber layer.
3. Bandgap alignment effects across the four absorber materials.

3.1 Limitations of the Model

The simulations assumed uniform optical generation rather than wavelength-dependent absorption. Perovskite-specific effects such as ion migration, hysteresis, and degradation were excluded. Series and shunt resistances were adjusted to reproduce typical fill-factor ranges. Therefore, the calculated efficiencies represent calibrated trends rather than exact experimental values.

3.2 Table 1. Baseline Device Parameters and Simulated Performance Metrics

Solar Cell	Eg(eV)	Absorber Thickness	Majority Doping	VOC(V)	JSC(mA/cm²)	FF (%)	PCE (%)
c-Si (monocrystalline)	1.12 (indirect)	180 µm (wafer)	p-type, ~1×10^{16} cm^{-3}	0.70	38.0	82	21.8
CdTe (thin-film)	1.45 (direct)	3 µm	p-type, ~1×10^{14} cm^{-3}	0.85	28.5	78	18.9
CIGS (thin-film)	1.15 (direct, Ga≈30%)	2 µm	p-type, ~1×10^{15} cm^{-3}	0.73	34.5	80	20.2
Perovskite ($CH_3NH_3PbI_3$)	1.55 (direct)	0.5 µm (500 nm)	nominally intrinsic (~1×10^{15} cm^{-3})	1.09	24.6	80	21.5

4. Results and Discussion:

The simulated results show clear differences in the electrical behavior of the four photovoltaic technologies. Silicon produces the lowest open-circuit voltage, approximately 0.70 V, which is mainly related to its relatively small

bandgap of about 1.12 eV and recombination losses within the absorber. At the same time, its broad spectral response allows the device to generate a comparatively high photocurrent. The perovskite device, in comparison, provides a much larger VOC of about 1.09 V. This higher voltage is associated with its wider bandgap and relatively low non-radiative recombination. Its JSC is around 25 mA/cm², with the current being restricted by the absorption range associated with its bandgap.

The CdTe and CIGS devices show intermediate electrical characteristics. The CdTe model gives a VOC of approximately 0.85 V and a JSC close to 29 mA/cm², consistent with its bandgap of about 1.45 eV. The CIGS device, using a bandgap near 1.15 eV, produces a higher current density of approximately 35 mA/cm², while its VOC remains around 0.73 V [37]. The four simulated devices exhibit relatively similar fill factors, falling within the range of approximately 78–82%, because realistic resistance and recombination effects were incorporated into the models [38].

The shape of the simulated J–V curves also provides useful information about device behavior. The perovskite cell maintains a relatively square-shaped curve over a broad voltage range, indicating efficient carrier collection and comparatively low recombination losses before reaching VOC. Silicon retains a strong photocurrent but shows a more gradual change in current near its operating voltage. CdTe and CIGS display some deviation from the ideal rectangular J–V shape, suggesting additional losses associated with resistance, interfaces, or carrier extraction. In the CdTe model, this behavior can be linked to limitations at the rear contact, whereas the CIGS device maintains good current generation but experiences a larger voltage loss relative to its bandgap. Overall, the comparison highlights the different factors governing voltage and current generation in each technology.

Comparative J–V Characteristics:

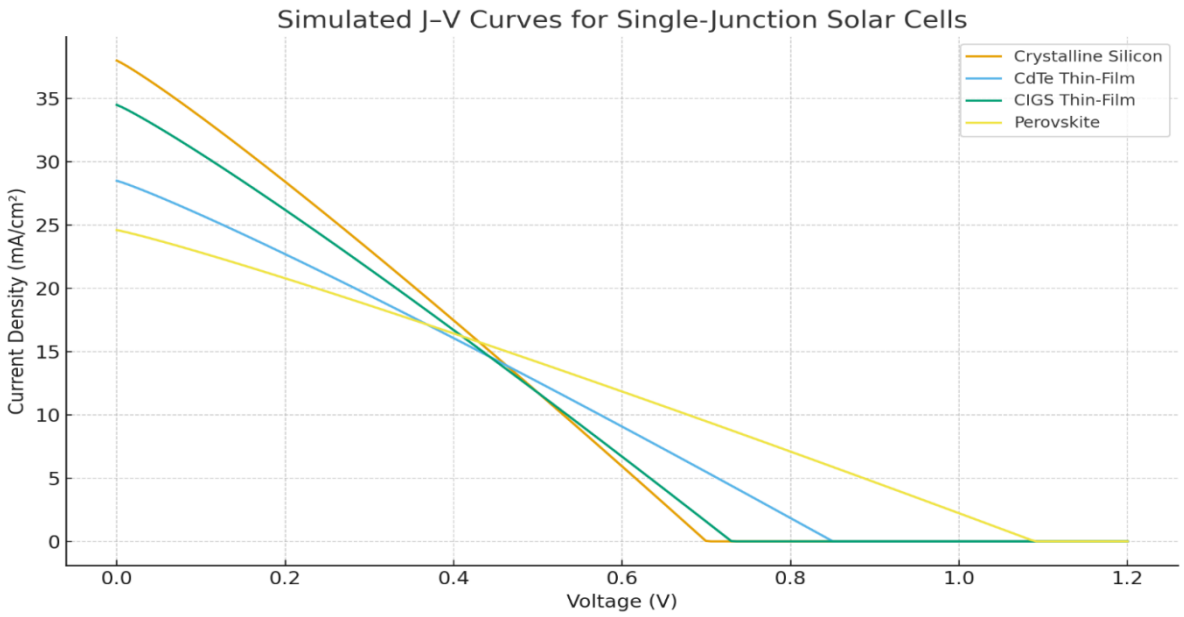

Figure 1: *Simulated J-V curves of representative single-junction solar cells, crystalline silicon (blue), CdTe thin-film (red), CIGs thin-film (green), & Perovskite (magenta). Each of the curves are plotted to 1s illuminated conditions and 25C using parameters from Table 1.*

The results presented in Figure 1 and Table 1 provides several important insights into the role of absorber bandgap and optical absorption in determining the balance between short-circuit current density (JSC) and open-circuit voltage (VOC). Materials with smaller bandgaps generally absorb a wider portion of the solar spectrum and can generate higher current, whereas wider-bandgap absorbers tend to support higher output voltages. The absorption coefficient also determines the thickness required for efficient light harvesting. CdTe, with a direct bandgap of approximately 1.45 eV, can achieve a JSC of around 29 mA/cm² using an absorber only a few micrometers thick. In

contrast, crystalline silicon requires a substantially thicker absorber because of its indirect bandgap and weaker optical absorption. A very thin silicon layer, without effective light trapping, absorbs only a limited portion of the incident solar radiation, demonstrating the optical advantage of direct-bandgap materials such as CdTe and perovskites [55].

CIGS provides a useful compromise between current generation and voltage. In the present simulation, the CIGS device with an Eg of approximately 1.15 eV produced a JSC of about 35 mA/cm² and a VOC near 0.73 V. Its direct-bandgap nature allows efficient operation with a relatively thin absorber. However, the difference between the bandgap and output voltage corresponds to a voltage deficit of approximately 0.42 V. Similar voltage losses have been reported in high-efficiency CIGS devices, indicating that recombination remains an important factor limiting further performance improvement [26].

The perovskite device exhibits a considerably higher VOC of approximately 1.09 V because of its wider bandgap and relatively low non-radiative recombination. Nevertheless, a noticeable voltage loss remains for an absorber bandgap near 1.55 eV. Further reductions in defect-assisted recombination through improved surface and interface passivation could provide additional improvements in VOC[39].

CdTe shows a comparatively large voltage deficit. For a bandgap of approximately 1.45 eV and a simulated VOC of about 0.85 V, the voltage loss is close to 0.60 V. This limitation is commonly associated with bulk defects, difficulties in achieving effective p-type doping, Fermi-level pinning, and recombination at the back contact [40]. Improvements in rear-interface engineering, including Te-rich layers and alternative buffer materials such as MgZnO or ZnTe, have been investigated to reduce these losses. The slight J–V rollover obtained in the CdTe simulation is also consistent with carrier-extraction limitations associated with non-ideal back contacts [41].

Thickness Dependence (Perovskite Case Study): One of the major advantages of perovskite and other direct-bandgap absorber materials is their ability to absorb sunlight efficiently using very thin active layers. To examine this characteristic, the influence of $CH_3NH_3PbI_3$ absorber thickness on perovskite solar-cell performance was investigated over the range of 0.1–1.0 μm (100–1000 nm). The variation in power conversion efficiency (PCE) is presented in Figure 2, while the corresponding values of VOC, JSC, and fill factor (FF) at selected thicknesses are summarized in Table 2.

The simulation shows a substantial increase in JSC as the absorber thickness increases from 100 nm to approximately 400–600 nm. At a thickness of 0.1 μm, the simulated current density is around 15 mA/cm², whereas it increases to approximately 24 mA/cm² near 0.4 μm. This improvement occurs because a thicker perovskite layer absorbs a larger fraction of incident photons and consequently produces more photogenerated charge carriers. The strong absorption coefficient of $CH_3NH_3PbI_3$ enables most above-bandgap radiation to be absorbed within only a few hundred nanometers [14].

In contrast to JSC, the open-circuit voltage shows a gradual reduction as the absorber becomes thicker. In the present simulation, VOC decreases from approximately 1.115 V at 100 nm to about 1.09 V at 400 nm and approaches 1.07 V at larger thicknesses. This behavior can be explained by the increase in bulk recombination pathways as the volume of the absorber increases. Although a thicker layer generates more carriers, carriers produced farther from the collecting contacts have a greater probability of recombining before extraction.

A similar trend is observed for the fill factor. The FF remains relatively high at moderate thicknesses but gradually decreases for thicker absorber layers because of increased carrier-transport and recombination losses [60]. As a result, increasing thickness does not continuously improve overall efficiency.

The combined effect of these competing factors produces an optimum perovskite thickness of approximately 400–600 nm under the simulated conditions. The maximum PCE of about 21–21.5% is obtained within this range, with the best performance occurring near 0.5 μm. Beyond approximately 0.8 μm, only small improvements in JSC are achieved, while reductions in VOC and FF begin to lower the overall efficiency. Previous experimental and simulation studies have reported similar behavior, where insufficient thickness limits light absorption, whereas excessively thick

films increase recombination and transport losses [14,60]. Thus, the results indicate that careful optimization of absorber thickness is essential for achieving high-performance perovskite solar cells.

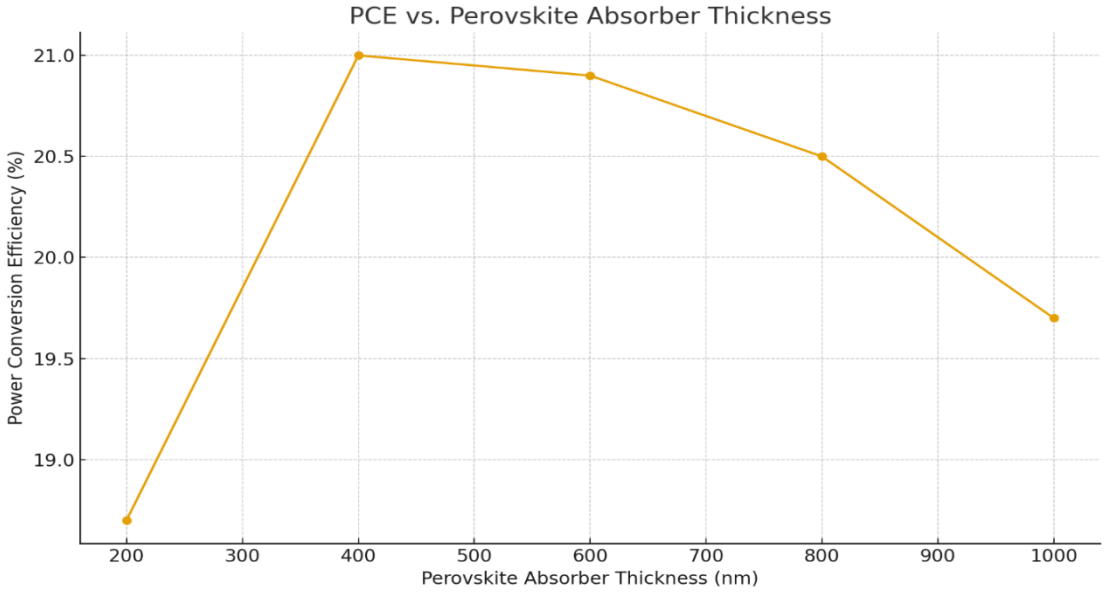

Figure 2. Maximum device performance is obtained when the perovskite absorber thickness is approximately 400–500 nm, producing a peak power conversion efficiency of about 21%.

Table 2. Variation of VOC, JSC , FF, and PCE with Perovskite Absorber Thickness

Perovskite Thickness	VOC (V)	JSC(mA/cm²)	FF (%)	PCE (%)
0.2 µm (200 nm)	1.10	21.2	80.0	18.7
0.4 µm	1.09	24.1	80.0	21.0
0.6 µm	1.08	24.5	79.5	20.9
0.8 µm	1.07	24.6	77.9	20.5
1.0 µm	1.06	24.63	75.0	19.7

4.1 Effect of Absorption, Defects, and Interface Quality on Device Performance:

The simulation results demonstrate that the strong optical absorption of perovskite materials is one of their major advantages. A $CH_3NH_3PbI_3$ absorber with a thickness of approximately 0.5 µm can absorb most of the useful incident radiation and reach close to its maximum simulated efficiency. This behavior is particularly important when compared with crystalline silicon, which requires a much thicker absorber because of its indirect bandgap and comparatively weak absorption coefficient. Without effective light-trapping structures, even a 1 µm silicon layer absorbs only a limited fraction of the incident solar spectrum [55]. In contrast, perovskites can achieve efficient photon absorption within a few hundred nanometers. This low material requirement is attractive for lightweight photovoltaic devices, flexible solar modules, and tandem architectures. CIGS and CdTe also benefit from strong absorption and normally require absorber thicknesses of only a few micrometers, making them considerably thinner than conventional silicon wafers [18,24].

The thickness study also indicates that increasing the perovskite layer beyond approximately 400–500 nm does not provide a proportional increase in power conversion efficiency. Once most of the useful photons have already been absorbed, additional absorber thickness contributes relatively little to J_{SC}. At the same time,

carriers generated deeper inside the film have a greater chance of undergoing recombination before reaching the transport layers. Consequently, very thick perovskite films may experience reductions in VOC and FF. The optimum thickness obtained from the present simulation therefore represents a balance between photon absorption and charge-carrier collection.

4.2 Influence of Bulk Defects:

Besides optical absorption, the density of defects within the absorber has a strong effect on photovoltaic performance. Defect states can act as recombination centers and increase Shockley–Read–Hall (SRH) recombination. As the defect concentration increases, the lifetime of photogenerated carriers decreases, leading to losses in VOC, FF, and PCE. The present simulation clearly illustrates this relationship for the perovskite device.

At a relatively low defect concentration of approximately 10^{14} cm^{-3}, the calculated VOC reaches nearly 1.14 V, indicating that recombination losses are relatively small. When the defect density is increased to approximately 10^{17} cm^{-3}, VOC decreases to around 0.95 V, while the FF falls from nearly 81% to 72%. Such changes produce a substantial reduction in the overall conversion efficiency. The results therefore suggest that maintaining the absorber defect density near 10^{15} cm^{-3} or lower is desirable when aiming for a VOC above 1.15 V in a perovskite material with a bandgap close to 1.55 eV.

Defect passivation is consequently an important strategy for improving perovskite devices. Various approaches, including the use of potassium iodide, formamidinium iodide, phenethylammonium-based compounds, polymers, and fullerene-related materials, have been investigated to reduce electrically active defects and suppress recombination. Such treatments can improve both VOC and FF by reducing the number of pathways through which electrons and holes recombine. The results obtained from the present defect-density analysis are consistent with this general behavior [39].

Perovskites also show a degree of tolerance toward certain intrinsic defects. Some native defects may generate relatively shallow electronic states and therefore have a smaller effect on non-radiative recombination than deep-level defects. This characteristic partly explains why high-quality polycrystalline perovskite films can achieve good photovoltaic performance despite containing more structural imperfections than high-purity crystalline silicon. Silicon devices, by comparison, require exceptionally low defect concentrations and long minority-carrier lifetimes to maintain high efficiency. Deep-level impurities or metallic contamination can significantly reduce carrier lifetime and voltage.

CdTe and CIGS generally contain higher defect concentrations than high-quality crystalline silicon, but their device structures can reduce the influence of these defects. Grain-boundary passivation, suitable doping, and optimized interfaces can improve carrier collection and reduce recombination. Nevertheless, defect-related voltage losses remain important limitations in these thin-film technologies [26,40].

4.3 Role of Interface Defects:

The quality of the interfaces between the absorber and charge-transport layers is another major factor affecting device performance. Interface defects can provide additional recombination centers and may also interfere with carrier extraction. In the present simulations, a high density of interface defects was found to produce distortions in the J–V characteristics, including an S-shaped response, together with reductions in VOC and FF. These effects are particularly important in heterojunction devices such as perovskite and CIGS solar cells.

The perovskite/ETL interface is especially sensitive to recombination. Earlier studies have shown that losses at the TiO_2/$CH_3NH_3PbI_3$ interface can strongly influence the device voltage [18,19]. A similar trend was obtained in the present simulation: increasing the perovskite/ETL interface recombination velocity by approximately 100 times reduced VOC by nearly 50 mV. This result highlights the importance of controlling interface defects and surface states. Surface passivation, thin insulating layers, and improved deposition processes can therefore play an important role in reducing interfacial losses.

The selection of the electron-transport layer also influences this behavior. Although TiO_2 has been widely used in perovskite solar cells, its interface with the absorber may contain states that promote recombination. SnO_2 has become an attractive alternative because of its favorable electronic characteristics and relatively low density of interfacial states. Its use has contributed to improved voltage and reduced hysteresis in many perovskite device structures [63].

Interface engineering is equally important for CdTe. Recombination at the CdTe/back-contact interface can reduce carrier extraction and cause losses in both VOC and FF. Incorporating suitable interfacial materials, such as Te- or ZnTe-based layers, or employing an appropriate high-work-function contact can reduce the barrier for hole extraction and suppress back-surface recombination [9]. In the present CdTe model, replacing the non-ideal rear contact with an ideal ohmic contact increased VOC by approximately 30 mV and FF by about 4 percentage points, producing an absolute PCE improvement of nearly 1.5%. Similar improvements in fill factor have been reported through optimized back-contact engineering, including the suppression of rollover or S-shaped features in the J–V characteristics [41].

Overall, the results show that strong absorption alone is not sufficient to obtain high photovoltaic efficiency. The best performance requires a suitable absorber thickness together with low bulk defect density and well-passivated interfaces. For perovskites, these factors are particularly important because their thin absorber layers provide excellent optical absorption but can become sensitive to bulk and interface recombination. The combined optimization of thickness, defect concentration, transport layers, and contact properties can therefore provide a practical pathway toward higher VOC, FF, and PCE across perovskite, CdTe, CIGS, and silicon solar-cell technologies.

Effect of Doping, Series Resistance, and Device Optimization

The electrical properties of a solar cell are strongly influenced by the doping level of the absorber and charge-transport layers. Doping changes the carrier concentration, depletion width, built-in electric field, and quasi-Fermi-level separation, thereby affecting the main photovoltaic parameters. In crystalline silicon, relatively high doping is normally used in the emitter and back-surface-field regions, whereas excessive doping in the base can increase Auger recombination and reduce carrier lifetime. Therefore, an intermediate base concentration is generally preferred for achieving a balance between voltage and current generation [18,64].

In the present silicon simulation, increasing the base doping concentration from **10^{15} to 10^{17} cm^{-3}** produced only a modest increase in VOC of approximately 10 mV. At the same time, JSC decreased by a few mA/cm^2 because of increased recombination and changes in the depletion region. Consequently, the overall efficiency showed little improvement. This result illustrates that increasing the doping level does not continuously enhance device performance. Beyond an appropriate concentration, recombination losses can offset the benefits associated with increased built-in potential.

A different behavior was obtained for the perovskite absorber. Perovskite layers are commonly treated as lightly doped or nearly intrinsic in device models. Introducing relatively high n-type doping in the range of **10^{16}–10^{17} cm^{-3}** resulted in a small reduction in simulated performance, mainly through a decrease in VOC. Additional free carriers can increase recombination while providing limited improvement in conductivity because high-quality perovskite films already possess suitable carrier-transport properties [18,64]. These observations support the use of appropriately doped transport layers rather than heavily doping the perovskite absorber itself. Asymmetric doping of the electron- and hole-transport layers can provide the required internal electric field for effective carrier separation [36].

The doping and mobility of the transport layers are particularly important for maintaining a high fill factor. For example, the Spiro-OMeTAD hole-transport layer requires adequate carrier concentration and mobility to minimize resistive losses. In the present model, a doping concentration of approximately **10^{18} cm^{-3}** and a mobility of **2×10^{-4} $cm^2/V \cdot s$** provided efficient hole transport. Reducing the doping concentration to approximately 10^{16} cm^{-3} resulted in a noticeable decline in FF because of increased transport resistance. Similar studies have identified an optimum range

of transport-layer conductivity for achieving efficient perovskite devices. Conductivity-enhancing additives such as Li-TFSI are commonly employed to improve the electrical properties of Spiro-OMeTAD [36].

Influence of Series Resistance:

Series resistance is another important parameter affecting solar-cell efficiency. It originates from the resistance of the absorber, transport layers, transparent conducting electrodes, metallic contacts, and other parts of the current-collection pathway. A higher series resistance reduces the slope of the J–V curve near the maximum-power region and generally lowers the fill factor. At high current densities, the effect becomes more pronounced and can also reduce the useful photocurrent.

For the comparative simulations, the series resistance was adjusted to produce realistic FF values close to **80%**. Silicon benefits from its high electrical conductivity and can achieve very low resistive losses, supporting fill factors above approximately 78% in high-performance devices [51]. Perovskite solar cells may experience somewhat larger resistive losses because of the properties of their transport layers and electrodes, although optimized devices can also achieve FF values above 80% [12]. CdTe and CIGS devices have historically experienced additional resistance associated with contacts and transparent conducting layers, but improvements in electrode design and current collection have progressively reduced these losses.

The simulation further indicates that eliminating series resistance would substantially improve the fill factor of all four technologies. Under an idealized zero-resistance condition, the calculated FF values increased toward the mid-80% range. This result demonstrates that contact engineering, transparent conducting layers, and transport-layer optimization remain important for obtaining high-performance devices. Minimizing resistive losses is therefore necessary for moving practical solar cells closer to their theoretical operating limits [18,51].

Overall Comparison and Design Implications:

The combined SCAPS-1D analysis provides useful information about the parameters controlling the performance of silicon, CdTe, CIGS, and perovskite solar cells. For perovskites, the results indicate that strong absorption allows the use of an absorber thickness of approximately **0.5 µm**, while defect density and interface recombination remain major limitations. Reducing the trap concentration toward the **10^{14}–10^{15} cm^{-3}** range can substantially improve VOC and FF by suppressing non-radiative recombination. These findings highlight defect passivation and interface control as important routes for further improvement.

Silicon, on the other hand, is already operating close to the practical limit of single-junction technology. Its indirect bandgap requires a relatively thick absorber, and further improvements are increasingly dependent on better surface passivation, contact selectivity, and advanced architectures. Tandem structures provide an especially promising pathway because they can combine silicon with a wider-bandgap absorber and utilize a broader portion of the solar spectrum [13].

CdTe and CIGS have strong optical absorption and can therefore operate with much thinner absorber layers than silicon. Their principal limitations are more closely related to voltage losses, recombination, and interface quality. Improving rear contacts, grain boundaries, buffer layers, and absorber composition could therefore provide further gains. For CIGS, controlled bandgap grading and alkali-metal treatments offer additional possibilities for improving carrier collection and reducing recombination.

Overall, the comparison shows that each technology requires a different optimization strategy. Silicon benefits mainly from contact and tandem development, CdTe from improved interfaces and rear-contact engineering, CIGS from bandgap grading and defect control, and perovskites from continued reduction of bulk and interface defects. Device-level simulations are valuable in this context because they allow individual parameters to be varied systematically before experimental fabrication, helping researchers identify the conditions most likely to produce meaningful improvements in photovoltaic performance.

Conclusion and Key Findings:

The comparative SCAPS-1D analysis provides a clear understanding of how the choice of absorber material and important device parameters affects solar-cell performance. The results show that photovoltaic efficiency is not controlled by a single parameter; instead, it depends on the combined effects of bandgap, optical absorption, absorber thickness, defect concentration, doping, recombination, and interface properties.

The bandgap and absorption coefficient strongly influence the relationship between current and voltage. Perovskite materials offer a relatively wide bandgap and strong absorption, allowing them to generate a high open-circuit voltage while maintaining good current generation. CdTe and CIGS also benefit from their direct bandgap characteristics, which permit efficient absorption using comparatively thin absorber layers. Silicon provides excellent current generation because of its broad spectral response, but its indirect bandgap requires a much thicker absorber to achieve effective photon absorption.

The simulations further demonstrate that absorber thickness must be carefully selected for each material. The perovskite device reaches its best performance with a thickness of approximately **400–500 nm**, where sufficient sunlight is absorbed without introducing excessive recombination and transport losses. Under the simulated conditions, the maximum PCE approaches **21%**. Increasing the thickness beyond this range produces only a limited improvement in JSC, while VOC and FF tend to decrease. CdTe and CIGS require absorber layers of a few micrometers, whereas crystalline silicon generally needs a thickness of approximately 100–200 μm.

Another major finding is the importance of defect density. Defects inside the absorber and at interfaces provide pathways for non-radiative recombination, which can reduce VOC, FF, and overall efficiency. For the simulated perovskite device, maintaining the bulk defect concentration below approximately $\mathbf{1 \times 10^{15}\ cm^{-3}}$ produces noticeably better performance. This emphasizes the value of defect-passivation methods and improved film quality. Similar considerations apply to CdTe and CIGS, where grain boundaries and heterointerfaces can contribute significantly to recombination losses.

The analysis also shows that doping and band alignment must be optimized rather than simply increased. Excessive absorber doping may increase recombination and reduce carrier lifetime, whereas appropriate doping of the transport layers can improve conductivity and reduce resistive losses. Proper energy-band alignment between the absorber and charge-transport layers is equally important because unfavorable offsets can restrict carrier extraction and increase interfacial recombination.

From a technology perspective, each material presents a different pathway for further development. Silicon is already close to its practical single-junction efficiency limit, making tandem architectures, improved passivation, and contact engineering important routes for future progress. CdTe can benefit from better rear-contact design, defect control, and interface engineering. CIGS offers additional opportunities through bandgap grading, buffer-layer optimization, and reduction of recombination-related losses. Perovskites remain particularly promising because their strong absorption, suitable bandgap, and high performance can be achieved using extremely thin active layers. However, improving long-term stability and resistance to environmental degradation remains essential for their wider commercial adoption.

Overall, the study confirms that absorber thickness, defect density, doping concentration, recombination, and interface quality must be optimized together to obtain high photovoltaic efficiency. The comparative modelling approach provides useful guidance for selecting suitable material parameters and identifying the major loss mechanisms in different solar-cell technologies. Such optimization can contribute to the development of lightweight, efficient, and cost-effective photovoltaic systems and support the broader transition toward sustainable electricity generation in line with United Nations Sustainable Development Goal 7 (Affordable and Clean Energy).

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