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*Original Article*

# Simulation of Solar Cell using SCAPS 1-D and Effect of Thickness on Lead-Free Solar Cell Performance

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***Abstract -*** *The growing global energy demand necessitates the adoption of sustainable and non-conventional energy sources such as solar, hydropower, and biomass. This study focuses on the simulation of a perovskite solar cell, which is lead-free ($CH_3NH_3SnBr_3$), with the help of SCAPS-1D software, incorporating a $NiO_3$ Hole Transport Layer (HTL). SCAPS-1D provides reliable computational modelling based on validated research data. The proposed lead-free solar cell design offers minimal material layer thickness while achieving comparable or superior efficiency. Its flexibility enables easy installation and transport, making it cost-effective and environmentally safe. Simulation results demonstrate the Power Conversion Efficiency, called (PCE) of 32.14%, and fill factor (FF) of 81.45%, and a short-circuit current density (Jsc) of 52.93 mA/cm². The study further reveals that an increase in absorber layer thickness enhances efficiency and FF up to an optimal threshold, beyond which a sharp decline is observed. Variations in Fluorine-Doped Tin Oxide (FTO) and $NiO_3$ layer thicknesses exhibit a minor decrease in efficiency with a slight improvement in FF. These findings provide valuable insights into optimizing lead-free perovskite solar cell structures for enhanced photovoltaic performance.*

***Keywords -*** *SCAPS1-D, Simulation, Efficiency, Solar cell, Green energy.*

## 1. Introduction

With the increasing global energy demand, there is an urgent need to transition from conventional fossil fuel-based energy sources, such as petroleum, to sustainable and renewable energy alternatives, including wind, solar, and biomass energy.

Fossil fuel reserves are finite and are depleting at an accelerating rate, raising concerns regarding energy security, environmental degradation, and pollution. Green energy sources offer a viable solution as they are self-sufficient, sustainable, eco-friendly, and freely available [1].

Their widespread adoption is essential for meeting energy demands while mitigating environmental impact. This study focuses on solar energy, particularly organic lead-free solar cells. Conventional silicon-based solar cells, though widely used, are expensive, while lead-containing perovskite solar cells pose toxicity risks to both the environment and human health [2]. Lead (Pb), with an atomic number of 82, is a heavy metal naturally occurring in the Earth's crust at low concentrations, as depicted in Figure 1. Due to its high density compared to other common materials, lead exhibits distinct physical and chemical properties. Some key characteristics of lead include:

### *1.1. Technical Overview of Lead and Lead-Free Perovskite Solar Cells*

Lead (Pb), a heavy metal with an atomic number of 82, typically appears grey or greyish-black. It is a soft, malleable metal with a shiny surface and a relatively low melting point. Lead exists in multiple oxidation states, including -4, -2, -1, 0, +1, +2, +3, and +4. It is diamagnetic in nature and possesses three stable isotopes. Despite its utility in various industrial applications, lead is a known neurotoxin, with extensive studies highlighting its detrimental effects on human health and the environment.

**Fig. 1 Source (www.Britannica.com)**

Although solar panels themselves are not the primary source of lead contamination, improper disposal or prolonged exposure to environmental conditions can cause degradation, releasing lead particles into the air, water, and soil. Lead reacts readily with rainwater and other atmospheric components, leading to persistent environmental contamination. Once introduced, lead remains in the environment indefinitely [3]. Its toxic effects include neurodevelopmental impairment, kidney damage, and adverse impacts on soft tissues in both humans and animals. Additionally, lead exposure is associated with hypertension [4], skeletal disorders [5], reduced fertility, and metabolic conditions such as increased uric acid levels (Falcone-like syndromes) [6]. Haematological disorders, including anaemia due to lead's interaction with Red Blood Cells (RBCs), have also been reported [7]. Chronic exposure can result in neurological dysfunction, behavioral abnormalities, and reproductive health issues, particularly in pregnant women, where complications such as miscarriage, stillbirth, and fetal malformation have been documented. Occupational exposure to lead has been identified as one of the carcinogenic materials by the International Agency for Research on Cancer (IARC) [9], with additional reproductive concerns such as reduced sperm count and increased abnormal sperm morphology in men [10]. To mitigate these risks, lead-free perovskite solar cells have emerged as an environmentally compatible alternative. These solar cells, based on bulk heterojunction structures, demonstrate high stability (up to 10%) under real-world conditions, enhanced flexibility, and low processing temperatures [11]. With superior optoelectronic properties, perovskites exhibit a wide range of photovoltaic applications [12]. Theoretically, these thin-film solar cells can achieve efficiencies exceeding 30% [13]. The manner of lead-free solar cells consists of a sandwich-like heterojunction structure, where the absorber layer is situated in between the Hole Transport Layer (HTL) and the Electron Transport Layer (ETL), forming a semiconductor diode. These solar cells leverage conductive organic polymers for efficient light absorption and charge transport. Their lightweight nature, extended lifespan, and compatibility with glass substrates make them highly adaptable for numerous energy applications [14]. Additionally, double perovskite solar cells utilize a p-i-n inverted structure, further improving their performance and stability in optoelectronic devices [15].

### 1.2. Material Components in Lead-Free Organic Solar Cells

A lead-free organic solar cell is being simulated in this study.

**Table. 1 List of Materials**

| |
|---|
| $NiO_3$ |
| $CH_3NH_3SnBr_3$ |
| $TiO_2$ |
| FTO |

#### 1.2.1. $NiO_3$ (Nickel Oxide) – Hole Transport Layer (HTL)

Nickel oxide ($NiO_3$) serves as the hole transport layer by facilitating hole mobility while effectively blocking electron transport. It possesses a stable crystal structure and exhibits high chemical stability, making it a reliable HTL material. While Carbon Nanotubes (CNTs) have been explored as alternative p-type dopants, they exhibit a degree of parasitic absorption, which can negatively impact device efficiency [15].

#### 1.2.2. $TiO_2$ (Titanium Oxide) – Electron Transport Layer (ETL)

Titanium dioxide ($TiO_2$) functions as the electron transport layer, characterized by low electron mobility and a high density of hole vacancies. It plays a critical role in solar cell performance due to its efficiency and stability. $TiO_2$ is typically doped at the uppermost layer of the solar cell and has been widely used as a stable ETL in previous studies [16].

#### 1.2.3. $CH_3NH_3SnBr_3$ (Methylammonium Tin Tribromide) – Absorber Layer

Methylammonium tin tribromide ($CH_3NH_3SnBr_3$) is employed as the absorber layer, responsible for photon absorption and photocurrent generation. It serves as the core component of the thin-film solar cell. Previous studies have demonstrated that various $CH_3NH_3XBr_3$ compositions yield high and stable power conversion efficiencies [17]. While $CH_3NH_3PbBr_3$ is known as an effective light harvester [18], this study replaces lead (Pb) with tin (Sn) to eliminate toxicity while maintaining or improving efficiency. Over the past few years, significant advancements have been made in optimizing the absorber layer to enhance power conversion efficiency (PCE) and extend the operational lifespan of solar cells.

#### 1.2.4. Fluorine-Doped Tin Oxide (FTO) – Transparent Conductive Electrode

Fluorine-Doped Tin Oxide (FTO) functions as the transparent conductive substrate in solar cells. It is optically transparent and mechanically robust, playing a crucial role in preventing charge leakage. Organic polymers used in conjunction with FTO typically exhibit intrinsic structural disorder, resulting in broad absorption spectra, which contribute to improved photovoltaic performance [19].

### 1.3. Fundamental Mechanism of Organic Solar Cell Operation

According to Solarmer Energy Inc. (2009), achieving a Power Conversion Efficiency (PCE) of at least 10% is a critical benchmark for the commercial viability of solar cells [20]. For efficient charge transport in the active layer, a conjugated bond structure is essential. This ensures that carbon (C) atoms within the active layer procedure covalent bonds through a discontinuous or alternating arrangement of single/double or single/triple bonds. In organic photovoltaic systems, the electronic structure is defined by the Lowest Unoccupied Molecular Orbital (LUMO), and another term is the Highest Occupied Molecular Orbital (HOMO). The difference in energy between these two levels is denoted by the term bandgap. The formation of a p-n junction between p-type and n-type semiconductor materials induces bending in the conduction and valence bands. Photons having equal or greater energy than the bandgap are absorbed, leading to the generation of electron-hole pairs [20]. These excitons (electron-hole pairs) have an extremely short lifetime, typically lasting only a few picoseconds. The excitation process propagates in a cascading manner, efficiently managing the excess energy. Subsequently, charge separation occurs at the donor-acceptor interface, where the electron-hole pairs dissociate and migrate toward their respective electrodes for collection [21]. This charge transport mechanism ultimately results in the generation of a photocurrent, which is the fundamental principle of organic solar cell operation.

## 2. Methods

A thin-film solar cell is being simulated with the help of SCAPS-1D (Solar Cell Capacitance Simulator), a computational tool developed by the University of Gent, Electronics and Information Systems (ELIS), Pietersnieuwstraat, Gent, Belgium [22]. SCAPS-1D is designed for the numerical modelling of solar cells, allowing for the simulation of both homojunction and heterojunction device architectures. To obtain accurate and reliable results, all input parameters within the simulation must be carefully selected. SCAPS-1D operates based on Poisson’s equation for electrons and holes, enabling a comprehensive analysis of device performance. The software allows for the simulation of various critical parameters, including layer thickness, defect density, operating temperature, and quantum tunnelling effects. While most capable simulation tools can typically model 5–6 layers, SCAPS-1D supports the simulation of up to 7 distinct layers within a solar cell structure [23]. Figure 2 presents an overview of the SCAPS-1D software interface and its setup. The software also provides key output characteristics, including:

- Current-Voltage (J-V) Characteristics
- Spectral Response
- Capacitance-Voltage (C-V) Analysis
- Capacitance-Frequency (C-F) Analysis

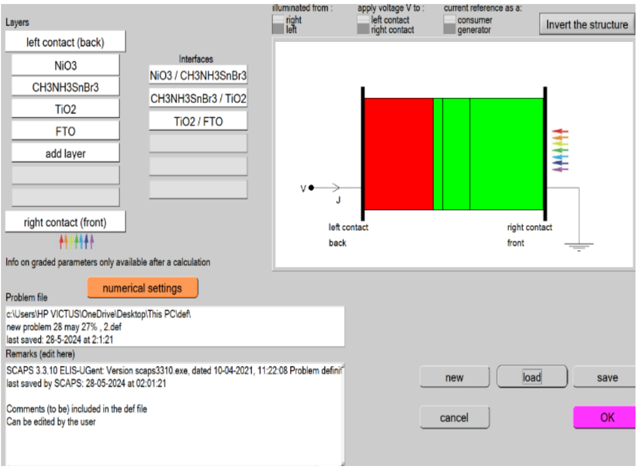

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**Fig. 2 Outlook ofSCAPS1-D software**

## 3. Result

Research conducted by R. Jayakumar, Atanu Bag, and their team analyzed the impact of material thickness on the solar cell efficiency and fill factor. Their study observed that increasing the thickness from 10 nm to 200 nm resulted in improved efficiency and fill factor. However, beyond this point, a decline in performance was noted due to increased recombination losses.

A separate study by Nima Khoshsirat determined that the optimal thickness for the buffer layer ranged between 40–50 nm, while the absorber layer thickness was found to be 2000–3000µm. Other studies suggested an absorber layer thickness of approximately 400 nm as optimal for efficiency. Experimental findings and previous research have consistently demonstrated that higher charge carrier mobilities within layers lead to greater efficiency. While thinner layers up to a certain thickness threshold enhance performance, excessive thickness increases charge carrier recombination, thereby reducing overall solar cell efficiency. Recombination shortens the lifetime of charge carriers as they undergo recombination before contributing to the current generation. Additionally, solar cells tend to exhibit better performance in high-temperature and humid environments. Various simulation parameters, such as voltage and temperature, were carefully selected to evaluate their influence on device performance. To systematically analyze the impact of thickness variation, simulations were conducted across all four layers of the solar cell. The corresponding graphs and simulation results deliver a deeper understanding about the relationship between layer thickness and overall efficiency. A detailed layer-wise thickness simulation is described in the following sections.

### *3.1. Effect of NiO₃ Layer Thickness on Solar Cell Performance*

A systematic simulation was conducted to analyze the impact of $NiO_3$ (Nickel Oxide) hole transport layer (HTL) thickness on solar cell efficiency and fill factor.

1. Increasing $NiO_3$ Thickness (Figure (3)):
    - When the thickness was increased from 1.300µm to 1.500µm, the efficiency improved from 31.76% to 32.14%, indicating a marginal enhancement in performance.
    - However, the fill factor (FF) slightly decreased from 81.37% to 81.25%, suggesting minor trade-offs in charge transport properties.

2. Decreasing $NiO_3$ Thickness (Figure (3)):
    - When the thickness was reduced from 1.500µm to 1.200µm, the efficiency exhibited a slight decline from 32.14% to 32.11%.
    - Conversely, the fill factor increased from 81.25% to 81.45%, indicating an improvement in charge collection efficiency.

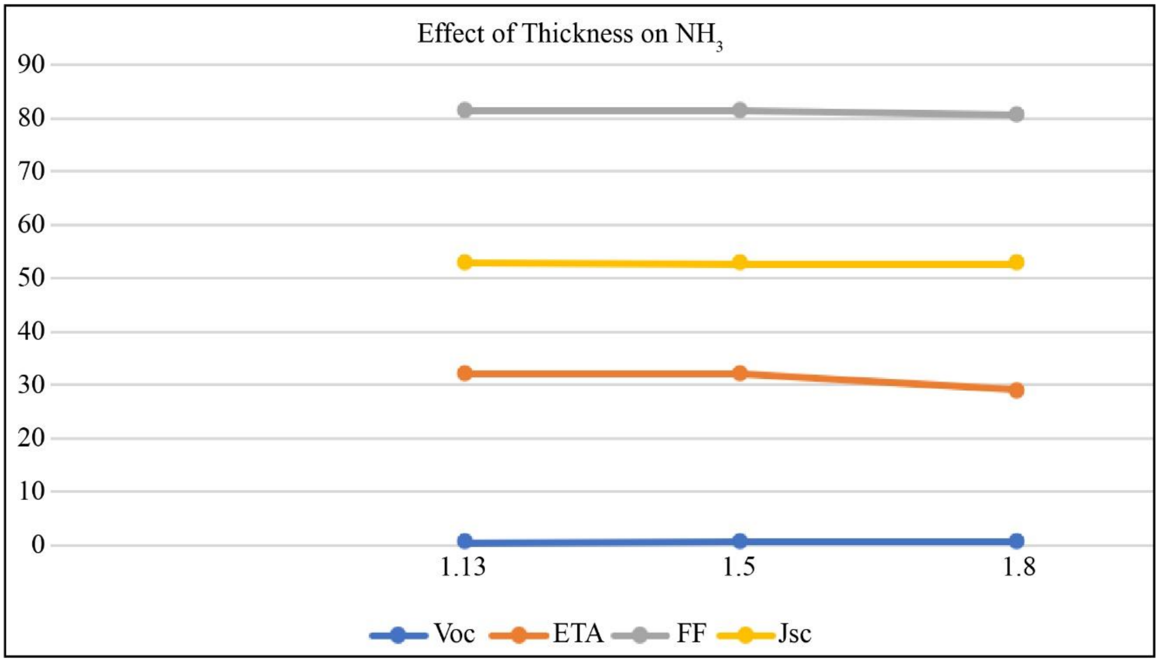

**Fig. 3 Thickness effect of NiO$_3$**

### *3.2. Effect of CH$_3$NH$_3$SnBr$_3$ Absorber Layer Thickness on Solar Cell Performance*

A detailed simulation was performed to assess the influence of CH$_3$NH$_3$SnBr$_3$ (Methylammonium Tin Bromide) absorber layer thickness on solar cell efficiency and fill factor.

1. Increasing CH$_3$NH$_3$SnBr$_3$ Thickness (Figure 4):
    - When the thickness was increased from 1.000µm to 1.150µm, the efficiency improved from 31.99% to 32.14%.
    - However, the fill factor exhibited a slight decrease, changing from 81.45% to 81.44%, suggesting minimal impact on charge extraction efficiency.
2. Decreasing CH$_3$NH$_3$SnBr$_3$ Thickness (Figure 4):
    - When the thickness was reduced from 1.150µm to 1.000µm, the efficiency declined slightly, from 32.11% to 31.99%.
    - The fill factor remained unchanged, indicating a negligible effect on charge transport properties.

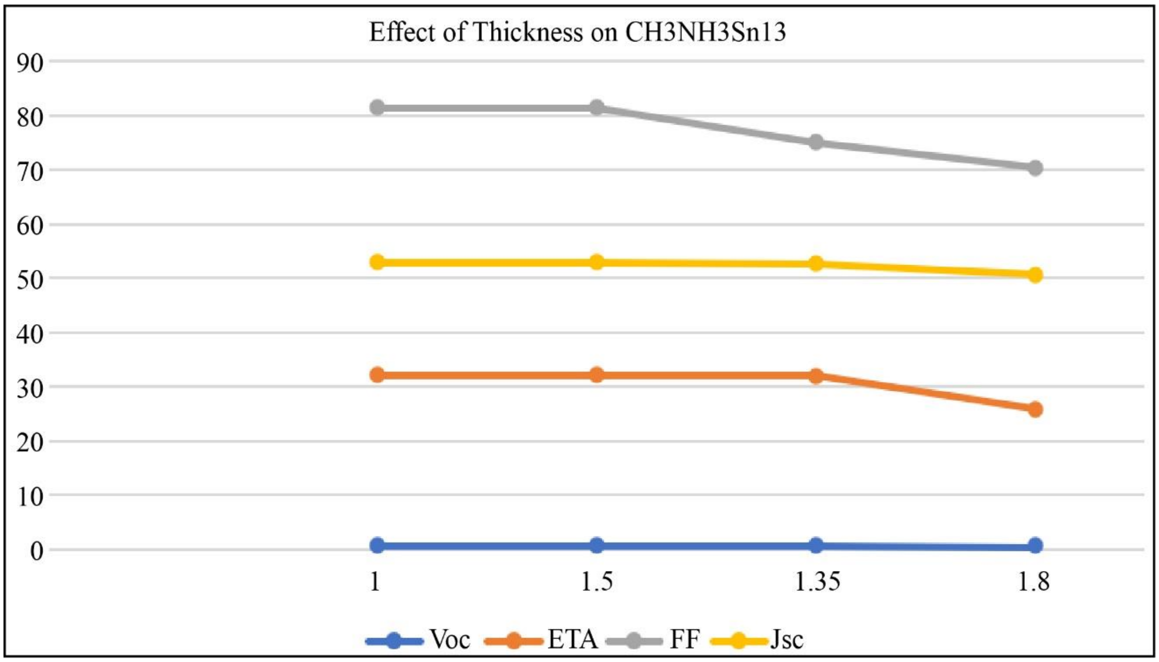

**Fig. 4 Thickness of active layer**

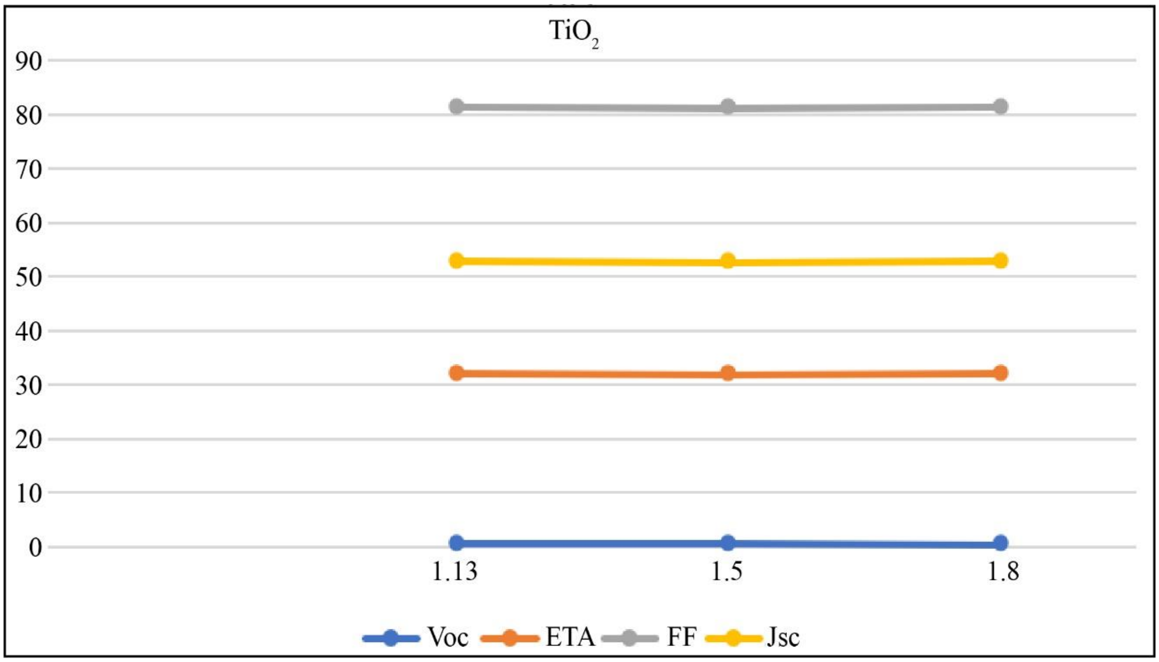

Fig. 5 Thickness of $TiO_2$

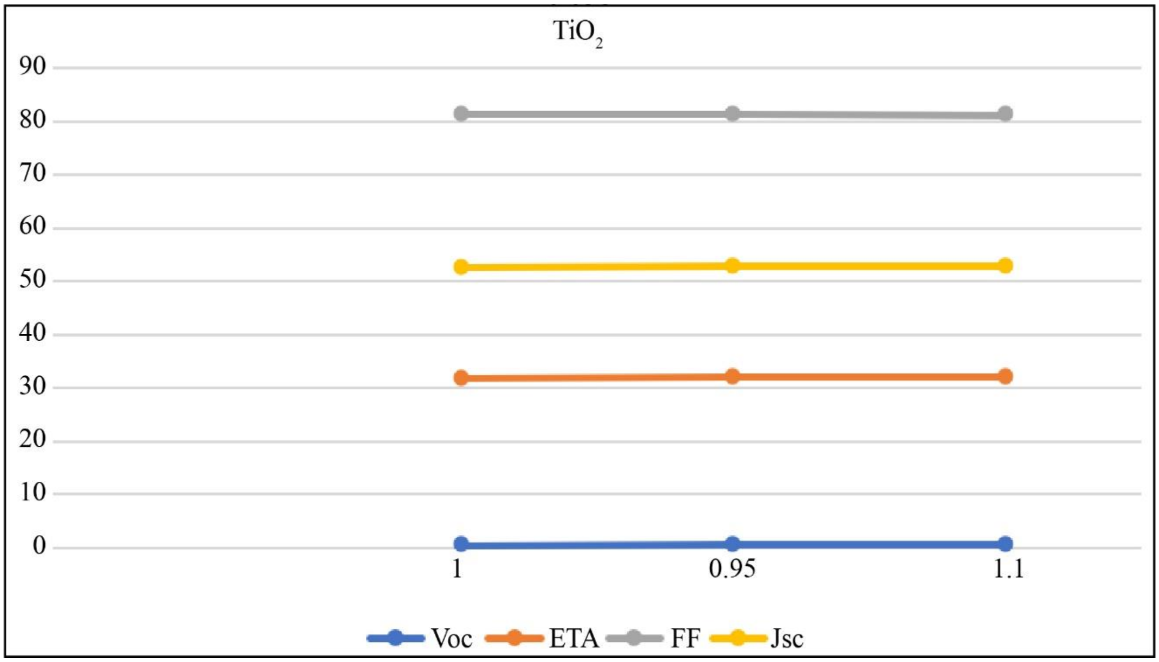

Fig. 6 Thickness FTO

### *3.3. Effect of $TiO_2$ Electron Transport Layer Thickness on Solar Cell Performance*

The influence of $TiO_2$ (Titanium Dioxide) electron transport layer (ETL) thickness on solar cell performance was analyzed through simulation.

1. Increasing $TiO_2$ Thickness (Figure 5):
    - When the thickness was increased from 0.8µm to 1.1µm, both the fill factor and efficiency remained unchanged, indicating minimal impact on charge transport and overall device performance.
2. Decreasing $TiO_2$ Thickness (Figure 5):
    - A similar observation was made when the thickness was slightly reduced, as neither fill factor nor efficiency exhibited any significant variation.

### *3.4. Effect of FTO Transparent Electrode Thickness on Solar Cell Performance*

The impact of Fluorine-doped Tin Oxide (FTO) transparent electrode thickness on solar cell efficiency and fill factor was analyzed through simulation.

1. Increasing FTO Thickness (Figure 6):
    - When the thickness was increased from 0.950 µm to 1.000 µm, the efficiency decreased from 32.14% to 31.91%, indicating a slight reduction in overall performance.

    - The fill factor remained unchanged, suggesting that the increased thickness primarily affected charge collection efficiency rather than transport properties.

2. Decreasing FTO Thickness (Figure 6):
    - When the thickness was reduced from 1.000 µm to 0.950 µm, the efficiency improved from 31.91% to 32.11%.

    - The fill factor showed a minor increase, from 81.44% to 81.45%, indicating a slight enhancement in charge extraction efficiency.

## 4. Conclusion

For achieving a high open-circuit voltage ($V_{oc}$) output, an extended non-radiative carrier lifetime is essential. In this study, all four layers were simulated under varying material thickness conditions while maintaining a constant temperature. The optimized simulation yielded a maximum efficiency of 32.14% and a fill factor (FF) in the range of 81.44%–81.45%. A short-circuit current density ($J_{sc}$) of 52.88%–52.93% was recorded, indicating stable charge generation and collection. Moderate increases in material thickness initially enhanced performance due to an increase in free-charge carriers. However, beyond a critical thickness threshold, efficiency sharply declined from 32.14% to 25%. This significant drop in efficiency is attributed to the increased hindrance in charge carrier transport, leading to higher recombination rates. While charge generation increases with thickness, excessive material thickness facilitates rapid recombination, reducing photocurrent output.

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