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Simulation And Optimization Of Perovskite Solar cells With Hybrid Electron Transport Layers Using SCAPS-1D Software

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KEDDAM & MENGEULLAT

خلاصة

وتمثل هذه الدراسة أن التكنولوجيا الجديدة التي تم تحليلها باستخدام برنامج محاكاة الخلايا الشمسية تمثل نجاحا في مجال الخلايا الشمسية. وقد أحدثت تحسينات كبيرة في التباين، البديل، والمتانة. وبفضل هذه التكنولوجيا، يمكن تحقيق زيادة كبيرة في تحويل الطاقة الشمسية إلى الكهرباء وخفض تكاليف الإنتاج بشكل كبير

وتمثل هذه واعدة جداً في مجال الطاقة الشمسية، حيث يمكن أن تساهم في استخدام الطاقة الشمسية بشكل أكثر فعالية وتنافسية كمصدر للطاقة النظيفة. من خلال تسهيل خصائص المواد والهياكل المبتكرة، يمكن لهذه التكنولوجيا أن تحدث ثورة في قطاع الطاقة الشمسية، مما يساعد في تقليل الاعتماد على الوقود الأحفوري والمؤثرات السلبية

Résumé

Ce mémoire explore l'impact d'une nouvelle technologie sur les cellules solaires, en se basant sur des simulations réalisées avec le logiciel SCAPS (Solar Cell Capacitance Simulator). Nous avons effectué une analyse approfondie des performances des cellules solaires, en examinant divers paramètres tels que l'efficacité de conversion, la stabilité et la durabilité. Les simulations ont permis d'identifier des améliorations significatives dans les propriétés des matériaux et des structures des cellules solaires. Les résultats de cette étude montrent des avancées prometteuses, suggérant que cette nouvelle technologie pourrait révolutionner le secteur de l'énergie solaire en augmentant l'efficacité et en réduisant les coûts de production.

Abstract

This thesis explores the impact of a new technology on solar cells, based on simulations conducted with the SCAPS (Solar Cell Capacitance Simulator) software. We conducted an in-depth analysis of solar cell performance, examining various parameters such as conversion efficiency, stability, and durability. The simulations allowed us to identify significant improvements in the material properties and structures of solar cells. The results of this study demonstrate promising advancements, suggesting that this new technology could revolutionize the solar energy sector by increasing efficiency and reducing production costs.

Summary

Chapter four : Simulation and optimization

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Symbols

V_{oc} : open circuit voltag

I_{sc} : Short-circuit current density

J-V : current voltage

I-V : electric current density

C-V : capacitance voltage

EQE : quantum efficiency

P_v : voltage power

P_{max} : Maximum power

FF : form factor

ɳ : Conversion efficiency

ETL : electron transport layer

HTL : hole transport layer

 : The potential

q : the elementary charge

ε : the permittivity

n : the density of free electrons

p : the density of free holes

Nd : the donor-type doping density

Na : the acceptor-type doping density

pt : the density of hole traps

nt : the density of electron traps

Gn (Gp) : the rate of optical generation of electrons (holes)

Rn (Rp) : the rate of recombination of electrons (holes)

Jn, J_p : the current densities of electrons and holes

SCAPS : solar cell capacitance simulator

General introduction :

The quest for clean and sustainable energy sources has long been a focal point of human innovation and progress. Among the myriad technologies vying for prominence in this domain, photovoltaic (PV) solar cells stand out as a beacon of hope, offering the promise of harnessing the abundant energy of the sun to power our world.

Solar energy, often hailed as the linchpin of a sustainable energy transition, is anchored by the fundamental technology of photovoltaic solar cells. These remarkable devices, capable of directly converting sunlight into electricity, represent the pinnacle of human ingenuity in our endeavor to create a cleaner and more sustainable future.

The journey of solar cells traces back through the annals of scientific discovery, from the pioneering work of Alexandre Edmond Becquerel to the groundbreaking advancements of Bell Labs and beyond. Each milestone in this saga has propelled us closer to realizing the full potential of solar energy as a viable alternative to fossil fuels.

At the heart of every photovoltaic cell lies the elegant phenomenon known as the photovoltaic effect, wherein solar photons trigger the release of charged electrons, generating an electric current. This intricate interplay of light and matter underscores the symbiotic relationship between nature's energy source and human technology.

In recent years, the emergence of perovskite solar cells has sparked a new chapter in the story of solar energy. These innovative devices, with their exceptional efficiency potential and low-cost fabrication, hold the promise of revolutionizing the solar landscape.

However, realizing the full potential of perovskite solar cells requires overcoming technical challenges and optimizing key components such as the Electron Transport Layer (ETL). By exploring hybrid ETLs and leveraging advanced simulation tools like SCAPS, researchers aim to enhance the performance and viability of these next-generation solar cells.

As we embark on this journey into the depths of solar cell technology, we delve into a world of innovation and possibility, where the fusion of science, engineering, and renewable energy promises to reshape the way we power our planet.

CHAPTER ONE

GENERAL INFORMATION ON PHOTOVOLTAIC SOLAR CELLS

Introduction

Solar energy, often presented as the key to a sustainable energy transition, is based on a fundamental technology, photovoltaic (PV) solar cells. These devices, capable of converting sunlight into electricity, embody the hope of a clean and renewable energy future. In this chapter, we will delve deeper into the generalities of solar cells, exploring their fascinating history, intrinsic composition, mechanism of operation, and the nuances of the benefits and challenges they offer in solar power production.

The saga of photovoltaic panels began well before the modern era, with precursors like Alexandre Edmond Becquerel, whose first discoveries of photovoltaic effects laid the foundations for this technology. Over the decades, pioneers such as Bell Labs and their famous silicon solar cells have marked important milestones in the development of solar panels, paving the way for the modern era of solar energy.

A photovoltaic solar cell is much more than just a device, it is the very embodiment of human ingenuity in its quest to harness the power of the sun. Basically, a photovoltaic solar cell is a semiconductor unit capable of directly converting sunlight into electricity, providing a clean and sustainable source of energy.

The innards of a solar cell reveal a complex world of semiconductors, doping and P-N junctions. Using materials such as crystalline or amorphous silicon, solar cells are meticulously designed to absorb solar photons, releasing charged electrons and holes that create an electric current.

At the heart of every photovoltaic cell is the photovoltaic effect, where solar photons act as energy messengers, exciting electrons in semiconductors and thus generating a flow of electric current. This ingenious process illustrates the perfect marriage between sunlight and human technology.

From their efficiency and durability to their size and cost, solar cells have a multitude of characteristics that shape their use in various applications. Their adaptability and efficiency are key elements in the transition to more widely deployed solar energy.

Solar power generation offers many benefits, from a reduced carbon footprint to increased energy independence. However, this is not without challenges, including variability in solar availability

and initial installation costs. Nonetheless, these challenges only highlight the importance of continued innovation in this area.

As we explore these generalities about solar cells, we will delve into a world of science, engineering, and hope for a cleaner, more sustainable energy future.[1]

1- History of photovoltaic panels :

The history of photovoltaic solar panels dates back to the 19th century, when the first concepts and experiments related to photovoltaic effects were developed. Below is a timeline of key events in the history of solar panels :

- **a- Photovoltaic Effect Discovered (1839)** : Alexandre-Edmond Becquerel discovered the photovoltaic effect when he observed that certain materials generate a small amount of electricity when exposed to light.
- **b- First Photovoltaic Cell (1883)** : Charles Fritts built the first solar cell based on selenium covered with a thin layer of gold. However, this first cell exhibited very low efficiency.
- **c- Photovoltaic Effect Explained (1905)** : Albert Einstein explains the photoelectric effect, laying the theoretical foundations for the conversion of light into electricity.
- **d- Silicon Cell (1954)** : Bell Labs produced the first silicon photovoltaic cell. This cell, developed by scientists Calvin Fuller, Gerald Pearson and Daryl Chapin, achieves an efficiency of 6%.
- **e- Space Applications (1958)** : The first solar panels are used in space. The Vanguard 1 satellite is equipped with solar cells to power its radio transmitters.
- **f- First Terrestrial Installations (1970)** : The first photovoltaic solar installations intended for the production of electricity for non-space use appear. They are mainly used in remote locations, far from traditional electricity networks.
- **g- Nobel Prize in Physics (1973)** : The Nobel Prize in Physics is awarded to the inventor of photovoltaic cells, Albert Einstein, as well as to William Shockley and Walter Brattain for their work on semiconductors.
- **h- 1980s Boom** : The 1980s saw a significant increase in the production and use of solar panels, largely due to the oil crisis and growing interest in renewable energy.
- **i- Cost Reduction (1990s)** : Technological advances and economies of scale lead to a reduction in the production costs of solar panels.
- **j- Recent Developments (2000s and beyond)** : Technological advancements continue with the introduction of new types of solar cells, such as thin-film solar cells and organic solar cells. The efficiency of solar panels is continually improving, and new applications.

The first photovoltaic cell (or solar cell) was developed in 1954 by researchers at Bell Labs in the United States, who discovered that the photosensitivity of silicon could be increased by adding "impurities".[1]

2- Definition of a PV solar cell :

The photovoltaic effect used in solar cells makes it possible to directly convert light energy from the sun's rays into electrical energy by generating and transporting positive and negative charges in semiconductor materials under the action of light.

3- Composition of a solar cell :

Photovoltaic solar cells are typically made of multiple layers of materials that work together to convert sunlight into electricity. The basic components of photovoltaic solar cells are:

- a- **Anti-reflective (AR) layer:** A thin layer applied to the surface of a solar cell to minimize the reflection of incoming light and allow more light to reach the active layer of the cell.
- b- **Transparent front layer:** Usually made of transparent glass or plastic, this layer allows light to enter the cell while protecting it from external influences.
- c- **Front Grille:** A transparent metal grille (usually silver in color) used to collect the electrical current produced by solar cells.
- d- **Semiconductor layer (usually silicon):** This layer is the active part of the solar cell and generates electron-hole pairs by absorbing sunlight. Depending on the crystal structure of silicon, solar cells can be monocrystalline, polycrystalline or amorphous.
- e- **PN junction (semiconductor junction):** A P (hole) junction and an N (electron) junction are formed in the semiconductor layer. These connections create an electric field that helps separate the charges generated by incident light.
- f- **Back grid:** A metal grid at the back of the cell that collects electrons released by absorption of light.
- g- **Reflective Lining:** A reflective layer on the back of a cell to minimize energy loss by reflecting light that is not absorbed as it passes through the cell.
- h- **Connector:** A metal connector that collects electricity generated by solar cells and transmits it to an external circuit.[2] [3]

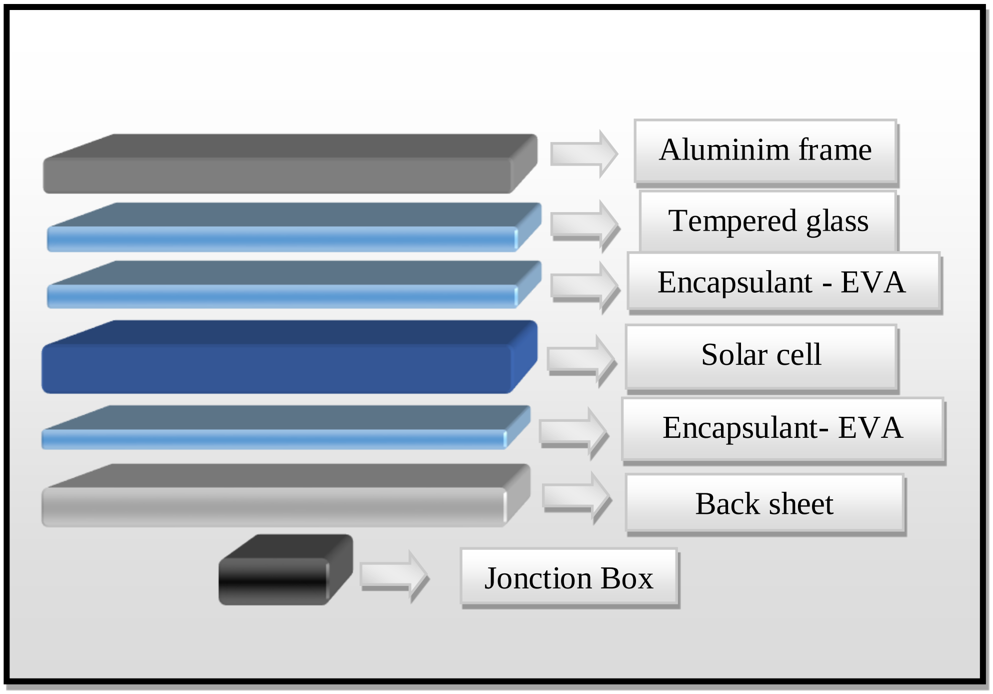


Figure 1.1 : the structure of photovoltaic module

5- The operating principle of a photovoltaic cell :

Photovoltaic cells work based on the photovoltaic effect, a phenomenon that occurs when sunlight hits something, usually a semiconductor, and produces an electric current. Here are the main stages in the operation of a photovoltaic cell :

a- Light absorption : Solar cells are made of semiconductor materials, mainly silicon. When sunlight hits the cell surface, it is absorbed by atoms in the material.

b- Formation of electron-hole pairs : The energy of a photon absorbs an electron from an atom of the semiconductor material, thus creating an electron-hole pair. Electrons have a negative charge, while holes lack electrons and represent a positive charge.

c- Movement of electrons and holes : Electrons excited by sunlight tend to move towards areas of the cell where the charge is negative, while holes move towards areas where the charge is positive. This movement creates a potential difference, also called voltage.

d- Charge separation : The internal structure of solar cells is designed to efficiently separate negative charges (electrons) and positive charges (holes). This prevents these charges from being trapped and recombining before creating a current.

i- **Current circulation :** An external circuit connected to the cell allows the current produced by the separation of charges to pass through it. This electricity can be used to power electrical equipment, charge batteries or integrate into the electricity grid.[3][4]

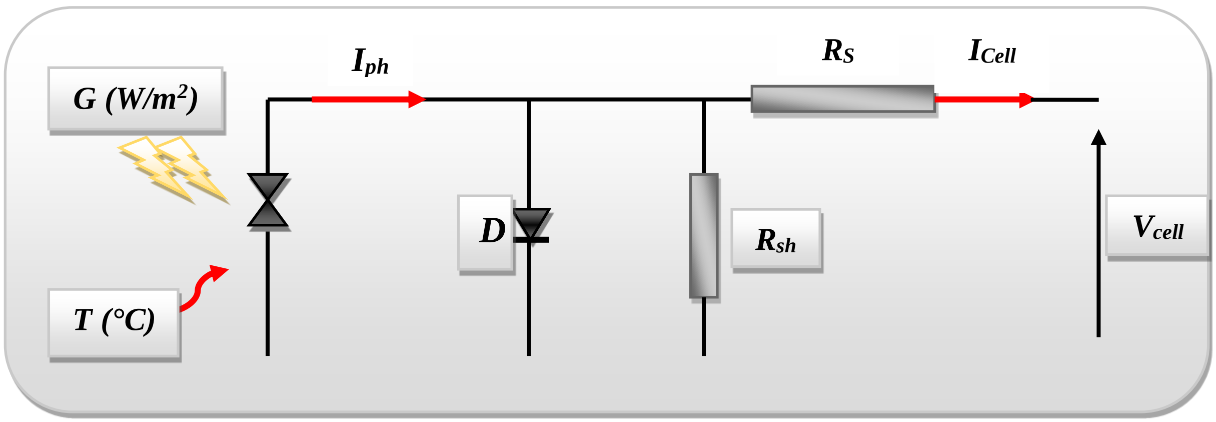


Figure 1.2: Equivalent electrical diagram of a photovoltaic cell

In summary The photovoltaic effect is the basis for the conversion of solar energy into electricity in solar cells. The efficiency of converting sunlight into electricity depends on various factors such as the quality of the semiconductor material, the design of the cell and the angle of incidence of the sunlight. When multiple solar cells are connected and encapsulated in a solar panel, they form a more powerful system capable of producing more electricity. These solar panels can be installed on roofs or above-ground structures, or integrated into various applications to provide a renewable energy source.

6- Various characteristics of solar cells :

The main characteristics that determine the operation and efficiency of solar cells are :

a- Open circuit voltage (V_{oc}) : Open circuit voltage is the voltage across the cell when no current is flowing. This is the maximum voltage available when the cell is exposed to sunlight and its terminals are not connected to an external circuit. For a cell solar ideal, there tension in circuit open East of:

$$V_{co} = \frac{KT}{q}\ln\left(\frac{I_{ph}}{I_s}+1\right) \approx V_{co} = \frac{KT}{q}\ ln\left(\frac{I_{ph}}{I_s}\right) \qquad (1)$$

b- Short-circuit current (I_{sc}) $Isc = (V = 0)$: Short circuit current is the current that flows through a cell when its terminals are short circuited. This is the maximum value of current that the cell can deliver under short circuit conditions.

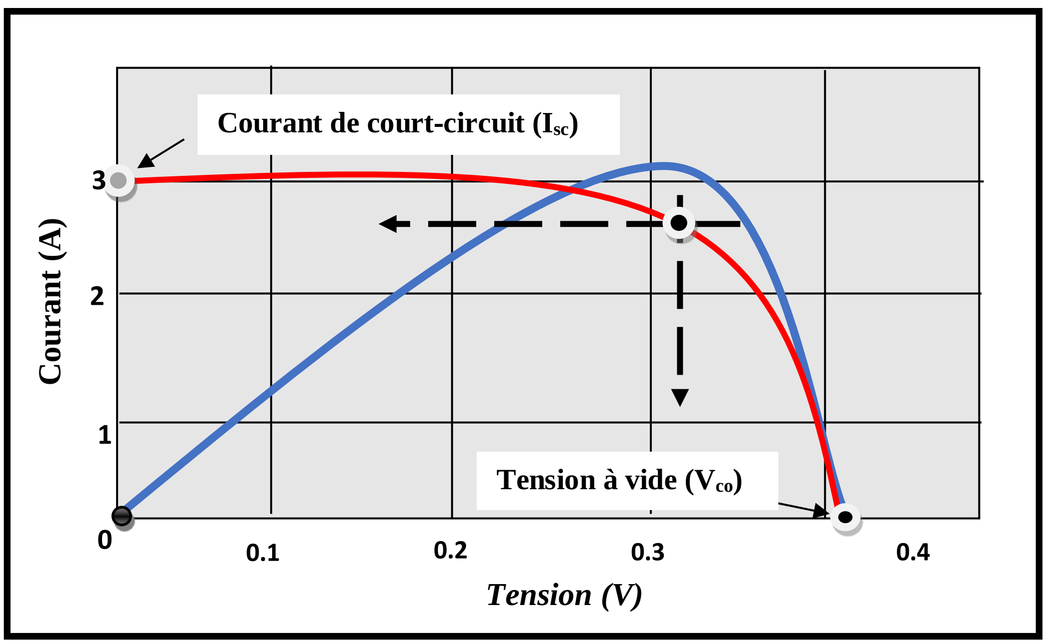


Figure 1.3 : curve of I = f (V)

c - Maximum power (P_{max}): The maximum power is the maximum power that the cell can deliver for a given light intensity. This is the result of multiplying the open circuit voltage by the short circuit current.

$$P_m = I_m . V \quad (2)$$

d - FF form factor : The normal operating point of a solar cell is the point on the I(V) curve which corresponds to the maximum power loss in the load. The form factor is called FF (Fill Factor):

$$FF = \frac{P_m}{I_{sc}.V_{co}} \quad (3)$$

e - Conversion efficiency : The efficiency of a solar cell is determined by the ratio between the power delivered at the maximum power point and the available light power.

$$\eta = \frac{P_m}{P_i} \quad (4)$$

Pi : is the incident power of solar radiation on the ground.

f - Temperature coefficient : The performance of solar cells changes with temperature. The temperature coefficient measures the variation in cell performance as temperature changes.

g - Spectral characteristics : The response of solar cells to light of different wavelengths can be different. Spectral characteristics describe how the cell responds to different parts of the solar spectrum.

h - Cell Types : There are several types of solar cells, including monocrystalline, polycrystalline and amorphous cells, each with unique advantages in terms of efficiency, cost and performance under certain conditions.[5][6][7]

Conclusion

In light of our exploration of the generalities of solar cells, it is clear that these photovoltaic devices are not simply technological components, but fundamental pillars of a global energy transformation. We have traveled a fascinating journey, from the initial discovery of the photovoltaic effect to modern innovations in solar cell design and manufacturing.

However, beyond the story, solar cells represent a beacon of hope in our quest for a more sustainable energy future. They offer the promise of clean, renewable energy, abundantly available and accessible to all.

Of course, challenges remain. Variability in solar availability, initial installation costs, and other technical hurdles must be overcome to fully realize the potential of solar cells. But these challenges only fuel our determination to innovate and progress.

In conclusion, solar cells are more than just a technology they embody our commitment to a cleaner, more sustainable and more equitable energy future for all. By continuing to invest in the research, development and deployment of solar cells, we can turn this vision into reality, delivering a brighter, more sustainable world for generations to come.

CHAPTER TWO

STATE OF THE ART OF CLASSIC AND PEROVSKITE SOLAR CELLS

Classic Solar Cells:

1. Introduction

Solar cells, or photovoltaic cells, convert sunlight directly into electricity and have become a cornerstone of renewable energy production. Since their inception, they have undergone significant advancements, becoming more efficient and cost-effective. This chapter provides an in-depth review of classic solar cell technologies, their operational principles, and the technological advancements that have driven their evolution.

2. Crystalline Silicon Solar Cells

2.1. Monocrystalline Silicon

Monocrystalline silicon solar cells are made from a single, continuous crystal structure. These cells are known for their high efficiency, often exceeding 20%, due to the high purity of the silicon used and the uniformity of the crystal structure. However, the manufacturing process is complex and costly, involving the Czochralski method to grow single-crystal silicon ingots. Despite the high initial cost, their superior efficiency and longevity make them a popular choice for residential and commercial installations.

2.2. Polycrystalline Silicon

Polycrystalline silicon solar cells are composed of silicon crystals that are melted together. While they are easier and cheaper to produce compared to monocrystalline cells, they typically exhibit lower efficiency, ranging from 15% to 18%. The reduced efficiency is due to the presence of grain boundaries that impede electron flow. Nonetheless, their lower production costs make them a widely used alternative in the solar industry. [8]

3. Thin-Film Solar Cells

3.1. Cadmium Telluride (CdTe)

CdTe solar cells are the most common type of thin-film technology. They consist of a thin layer of cadmium telluride deposited on a substrate such as glass or plastic. CdTe cells are cost-effective and can achieve efficiencies of around 10% to 12%. One of the major challenges with CdTe technology is the toxicity of cadmium, which poses environmental and health risks. Efforts are ongoing to recycle CdTe materials safely and to find safer alternatives.

3.2. Copper Indium Gallium Selenide (CIGS)

CIGS solar cells use a thin layer of copper, indium, gallium, and selenium. They offer higher efficiency compared to CdTe cells, typically ranging from 12% to 14%. CIGS cells are flexible and lightweight, which makes them suitable for a variety of applications, including building-integrated photovoltaics (BIPV) and portable solar devices. However, the scarcity and high cost of indium and gallium are significant drawbacks.

3.3. Amorphous Silicon (a-Si)

Amorphous silicon solar cells feature a non-crystalline form of silicon. These cells are less efficient (with efficiencies between 6% and 8%) but are cheaper to produce and can be deposited on flexible substrates. This flexibility makes them ideal for applications in consumer electronics and other niche markets. They also have better performance in low light conditions compared to crystalline silicon cells. [9]

4. Technological Advancements

Recent advancements in classic solar cell technologies focus on enhancing efficiency and reducing costs. Some of the notable innovations include:

- **Silicon Heterojunction Cells**: These cells combine crystalline and amorphous silicon layers, achieving efficiencies over 25%. The heterojunction design reduces recombination losses and enhances carrier collection.
- **Bifacial Solar Cells**: These cells can capture sunlight from both sides, increasing total energy output. They are particularly effective in installations where light can be reflected onto the rear side, such as on white rooftops or snow-covered ground.
- **Surface Passivation Techniques**: Improved surface passivation methods, such as using passivated emitter and rear cell (PERC) technology, have significantly reduced electron recombination at the surface, leading to higher efficiencies. [10]

5. Challenges and Future Prospects

Despite significant advancements, several challenges remain in the development of classic solar cells. Key areas of focus include:

- **Durability and Longevity**: Enhancing the lifespan of solar cells, particularly in harsh environmental conditions, is critical. Research is ongoing to develop more robust materials and protective coatings.

- **Recycling and Sustainability**: Addressing the environmental impact of solar cell production and disposal is crucial. Developing efficient recycling methods and using environmentally friendly materials are priority areas.
- **Cost Reduction**: Continued efforts to reduce manufacturing costs without compromising efficiency are essential to make solar energy more accessible and competitive with conventional energy sources.

Future research directions include exploring new cell architectures, such as multi-junction and tandem cells, which can achieve higher efficiencies by capturing a broader spectrum of sunlight. Additionally, the development of alternative materials that are abundant, non-toxic, and cost-effective will be crucial in overcoming current limitations. [11][12]

Conclusion

Classic solar cell technologies, particularly those based on crystalline silicon and thin-film materials, have made significant strides in efficiency and cost reduction. They remain at the forefront of the renewable energy revolution, with ongoing research and technological innovations promising even greater advancements. By addressing existing challenges and exploring new frontiers, solar cells have the potential to play a pivotal role in the global transition to sustainable energy.

Perovskite solar cells:

Introduction

Perovskite solar cells have emerged as a revolutionary technology in the field of renewable energy over the past decade. With their unique properties and rapid progress in terms of performance and cost, they are attracting increasing interest in photovoltaic research and industry. This chapter presents a detailed state-of-the-art review of perovskite solar cells, covering their evolution, recent advances, technical challenges, and future prospects.

1. Historical Development and Evolution of Perovskite Solar Cells

Perovskite solar cells began to attract attention around 2009, with the use of hybrid organic-inorganic perovskites as active materials in photovoltaic devices. Initially, the first cells exhibited modest energy conversion efficiencies of around 3.8%. However, a series of discoveries and optimizations quickly increased the efficiency to over 25% in less than ten years.

1.1 Early Generations

The early generations of perovskite cells used simple structures with perovskites such as CH3NH3PbI3 (methylammonium lead iodide). Major challenges included low stability and sensitivity to moisture.

1.2 Structural Optimizations

The introduction of new compositions, such as formamidinium (FA) perovskites and mixed anionic/cationic systems, improved the performance and stability of the devices. Additionally, multi-layer structures and tandem architectures were developed to maximize light absorption and minimize losses. [13]

2. Properties and Materials of Perovskite Solar Cells

The perovskites used in solar cells are crystalline compounds with an ABX3 structure, where 'A' is an organic cation (such as methylammonium or formamidinium), 'B' is a metal (usually lead or tin), and 'X' is a halide (iodine, bromine, or chlorine).

2.1 Optoelectronic Properties

Perovskites are characterized by strong light absorption, high charge mobility, and long charge carrier diffusion lengths, making them extremely efficient for photovoltaic conversion.

2.2 Lead-Free Materials

Due to environmental concerns related to the use of lead, intensive research is being conducted to develop lead-free perovskites, such as tin-based (Sn) perovskites. [14]

3. Fabrication Techniques

The fabrication of perovskite solar cells relies on various techniques aimed at producing high-quality thin films.

3.1 Spin-Coating

Spin-coating remains one of the most common techniques for depositing perovskite layers, allowing precise control over film thickness and uniformity.

3.2 Solution Deposition Techniques

Solution deposition techniques, including the anti-solvent method and two-step deposition, are widely used to optimize the crystallization and morphology of perovskite films.

3.3 Large-Scale Manufacturing

For industrial production, techniques such as thermal evaporation and inkjet printing are explored for their compatibility with large-scale processes. [15]

4. Technological Advances

Recent advances aim to improve the efficiency and stability of perovskite solar cells.

4.1 Tandem Cells

Tandem cells, combining perovskites with other photovoltaic materials such as silicon, allow for record efficiencies by exploiting a broader range of the solar spectrum.

4.2 Interface Optimization

Improving the interfaces between the perovskite layer and charge transport layers is crucial for minimizing non-radiative recombination and maximizing charge extraction. [16]

5. Challenges and Solutions

Despite significant progress, several challenges remain for the commercialization of perovskite solar cells.

5.1 Stability and Durability

Perovskites are sensitive to moisture, heat, and UV light, affecting their long-term stability. Strategies such as encapsulation and chemical composition modification are being explored to enhance durability.

5.2 Scaling Up Production

Transitioning from laboratory production to large-scale manufacturing requires reproducible and economical processes. Optimizing deposition methods and reducing material costs are essential for this transition.

5.3 Environmental Impact

The presence of lead in perovskites poses toxicity concerns. Developing alternative materials and recycling protocols are active research areas to mitigate this impact. [17]

Conclusion

Perovskite solar cells represent a major advancement in photovoltaic technology, offering a promising combination of high efficiency and potentially low production costs. Continuous improvements in stability, large-scale manufacturing, and environmental impact reduction are crucial for their commercial adoption. Current and future research focuses on optimizing these aspects, making perovskite solar cells a key technology for the renewable energy landscape of tomorrow. [18] [19] [20]

CHAPTER THREE

PEROVSKITE MATERIAL

Introduction

This chapter explores the promising advancements in perovskite solar cells, a technology set to revolutionize photovoltaics. We begin by examining perovskite materials, known for their remarkable electronic and optical properties, making them ideal for converting sunlight into electricity. Understanding the crystal structure of these materials is crucial as it defines their unique capabilities.

Tracing the history of perovskite solar cells, we highlight key discoveries and developments that have shaped this technology. From its initial discovery to recent breakthroughs, we provide a comprehensive overview of its evolution.

We delve into the operating principles of perovskite solar cells, explaining the complex processes within these devices. This includes light-matter interactions and the generation and separation of charges, fundamental to transforming solar energy into electric current.

The chapter also covers the architecture and manufacturing processes of perovskite solar cells. We describe various approaches and techniques used to design and produce these devices, detailing each step from material preparation to final assembly.

Different structures and configurations of perovskite solar cells are explored, showcasing their respective advantages and limitations. This analysis provides insights into the design and engineering choices that make this technology promising.

Practical aspects of manufacturing a prototype perovskite solar cell are discussed, including necessary materials and equipment, and potential challenges in the production process.

We then address the advantages and limitations of perovskite solar cells. High efficiency and reduced costs are weighed against challenges such as long-term stability and sustainability.

Finally, we delve into the dynamic field of research and development, highlighting the latest advances and future prospects of perovskite solar cells. A detailed comparison between perovskite solar cells and traditional solar cells is provided, emphasizing key differences and implications for the future of solar energy.

1- Perovskite materials:

These perovskite materials are a family of crystalline compounds that take their name from the characteristic crystal structure of the perovskite mineral. Their crystal structure is generally face-centered cubic, with a particular arrangement of ions. This structural pattern gives them unique electrical and optical properties, particularly when used in photovoltaic applications.

This precursor are often composed of organic ions, such as methylammonium or formamidinium, associated with inorganic metal ions, such as lead, bismuth or cesium. They are valued for their wide range of sunlight absorption, allowing them to efficiently capture solar energy over a range of wavelengths.

Perovskites have several characteristics that make them particularly attractive for photovoltaic applications :

a- Wide Light Absorption :

Perovskites have a wide band gap, meaning they can efficiently absorb light across a wide range of wavelengths in the solar spectrum. This increased ability to capture sunlight improves their efficiency in converting light energy into electricity.

b- High Mobility of Charge Carriers :

In perovskites, electrons and holes generated by light absorption have high mobility, meaning they can move easily through the material to be collected at the solar cell's electrodes. This high mobility contributes to better performance of solar cells by allowing efficient collection of charge carriers.

c- Ease of Manufacturing :

Perovskites can be made from relatively simple precursor solutions and can be deposited on a variety of substrates, including flexible substrates. This ease of manufacturing provides great flexibility in the design and manufacturing of solar cells, which can reduce production costs and speed up the manufacturing process.

d- Potentially Reduced Costs :

Due to their relatively simple manufacturing and the abundance of some of their components, perovskite solar cells have the potential to reduce production costs compared to established photovoltaic technologies such as crystalline silicon. This cost reduction can help make solar energy more competitive in the energy market. [21] [22]

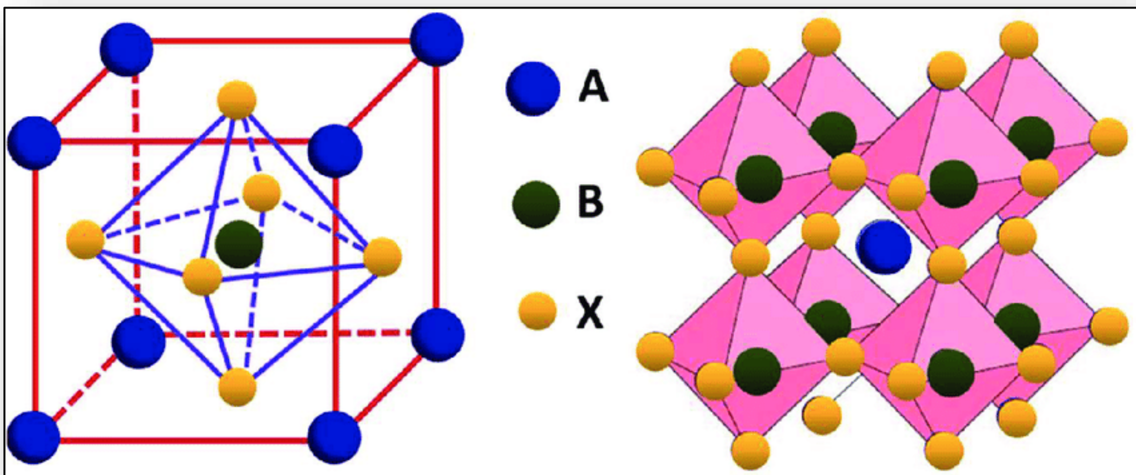


Figure 2.1 : Schematic of the crystal structure of perovskite materials

With elements A, B and X can be :

A : cation (Cs^+, Rb^+, MA^+, FA^+, ...),

B : cation (Pb^{2+}, Sn^{2+}, Ge^{2+}, ...),

X : anion (halides (I^-, Br^-, Cl^-,...)

2- History :

The history of perovskites in solar cells is relatively recent but very dynamic. Here is an overview of its evolution:

Start of Research: The first research into the use of perovskites in solar cells began in the 2000s, mainly due to their particular crystal structure and their high potential for converting sunlight into electricity.

2009 breakthrough: In 2009, Tsutomu Miyasaka and his team at the University of Tokyo published a groundbreaking study demonstrating the use of perovskites as a photoactive layer in solar cells. Their research laid the foundation for what would become a major breakthrough in solar energy.

Successive Yield Records: Since this discovery, researchers have worked on optimizing perovskites for solar cells, which has led to a dramatic increase in efficiencies. Records for perovskite solar cell efficiency have been steadily broken in recent years, quickly reaching levels comparable to established photovoltaic technologies such as crystalline silicon.

Expansion and Diversification: Interest in perovskites in solar cells has rapidly expanded across the global scientific community, with many research institutions and private companies investing in this area. In addition to increasing efficiency, researchers have also worked on the long-term stability of perovskites and reducing manufacturing costs to make this technology more competitive in the market.

Practical Applications: Perovskite solar cells are beginning to be used in practical applications, including rooftop photovoltaic installations and large-scale pilot projects. Collaborations between universities, research institutes and private sector companies aim to accelerate the commercialization of this technology and make it accessible to the general public.[23] [24]

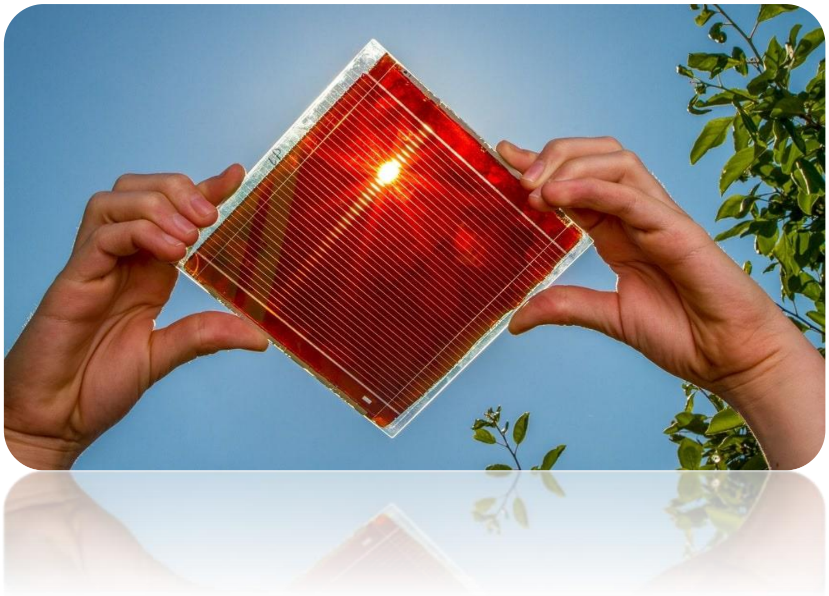


Figure 2.2 : Prototype of a perovskite solar plate

In summary, although the history of perovskites in solar cells is relatively short, it is marked by significant progress and major breakthroughs. With continued investment in research and development, perovskites have the potential to play an important role in the global transition to clean, renewable energy.

3- Operating principle of a perovskite solar cell :

- Perovskite solar cells work by exploiting the photovoltaic effect, a process by which sunlight is converted into electricity.
- At the heart of the perovskite solar cell is a thin layer of perovskite material that acts as the active conversion layer.
- When sunlight hits the solar cell, the perovskites absorb some of that light, thereby exciting the electrons in the crystal structure.
- Excitation of electrons creates electron-hole pairs, where an electron is released from its bond with an atom, leaving behind a positively charged hole.

- The excited electrons move to the perovskite layer where they are collected by one electrode, while the holes move to the other electrode.
- This movement of electrons and holes creates a flow of electrical current that can be collected by electrodes and used to power electrical devices or stored in batteries.

In short, perovskite solar cells use perovskite materials to directly convert light energy from the sun into electricity, through the creation of electron-hole pairs and the collection of charge carriers.[25]

4- Architecture and manufacturing of perovskit e cells:

a- Architecture of the perovskite solar cell :

- ***Active perovskite layer :*** This layer is the heart of the solar cell and is responsible for converting sunlight into electricity. Perovskites are deposited in the form of thin layers on a conductive substrate. They are typically composed of organic-inorganic perovskite crystals, such as methylammonium lead iodide (MAPbI3).
- ***Electron and Hole Transport Layers :*** The ETL and HTL layers are crucial to facilitate the efficient transfer of electrons and holes generated in the perovskite layer to the electrodes. ETL and HTL are typically composed of organic or inorganic conductive materials, such as TiO2 for ETL and Spiro-MeOTAD for HTL.
- ***Electrodes :*** The top (anode) and bottom (cathode) electrodes are responsible for collecting electrons and holes to generate an electric current. Commonly used electrode materials are indium tin oxide (ITO) or titanium dioxide (TiO2) for the anode, and aluminum or silver for the cathode.

d- **Manufacturing of perovskite solar cells** :

- ***Preparation of substrates** :* The substrates, generally glass or transparent and conductive plastic sheets, are cleaned and prepared to ensure good adhesion of the layers of active materials.
- ***Deposition of the perovskite layer** :* The perovskite layer is deposited on the substrate using techniques such as spin-coating, vacuum evaporation or inkjet printing. The perovskite precursor solution is deposited and then heat treated to form a crystalline layer.
- ***Deposition of electron and hole transport layers** :* The ETL and HTL layers are deposited on the perovskite layer to enable the efficient transfer of charge carriers. These layers can be deposited by techniques similar to that of the perovskite layer.
- ***Encapsulation** :* To protect the solar cell from moisture, contaminants and mechanical damage, it is encapsulated in protective materials such as glass or plastic, with seals to ensure long life.

c- Characterization and quality control :

- Perovskite solar cells undergo a series of characterization tests, including efficiency, stability and durability measurements, to evaluate their performance and reliability.
- Advanced techniques such as scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS) are used to characterize the structure and composition of perovskite layers and transport layers.
- Devices that meet the required quality standards are then integrated into solar modules for practical use in photovoltaic applications. [26] [27]

5- <u>Structure of the different architectures of Perovskite solar cells:</u>

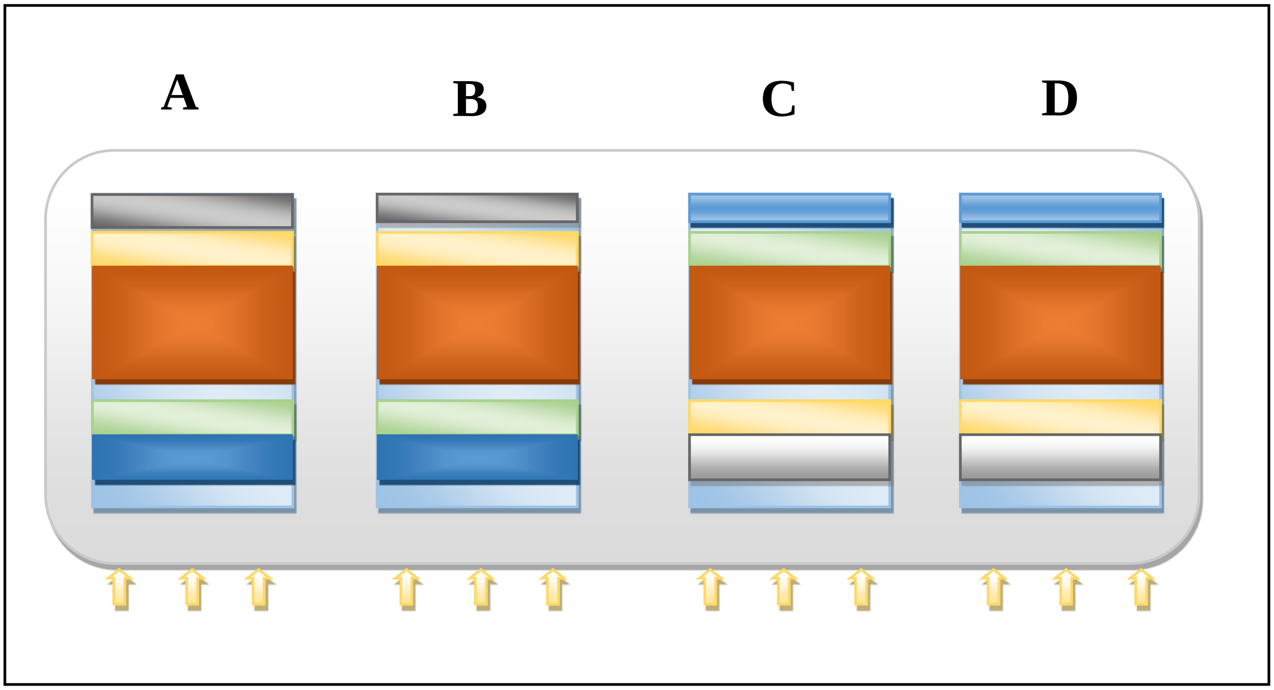
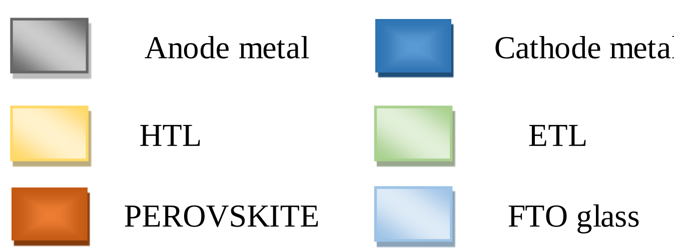


Figure 2.3 : Structure of the different architectures of Perovskite solar cells

- **(A):** NIP mesosporous structure
- **(B):** NIP planar structure
- **(C):** PIN planar structure
- **(D):** PIN mesosporous structure



6- Equipment required for the manufacture of a prototype of a perovskite solar cell :

To fabricate a perovskite solar cell prototype, you will need a set of specialized devices and equipment to handle and deposit the different materials, as well as to characterize the performance of the device. Here is a list of devices typically used for manufacturing a perovskite solar cell prototype:

a- **Controlled Atmosphere Gantbox:** To handle moisture and oxygen sensitive materials in an airless environment, a controlled atmosphere gantbox is often used.

b- **Centrifuge:** To mix the perovskite precursors and prepare the solutions to be deposited on the substrates, a centrifuge is necessary to obtain homogeneous coatings.

c- **Spin-coater** : To uniformly deposit the thin layers of perovskite on the substrates, a spin-coater is used. It allows you to control the rotation speed and spin time to obtain quality thin films.

d- **Vacuum Evaporator:** For the deposition of certain thin films such as electron or hole transport layers, a vacuum evaporator is used to deposit the materials in a controlled manner on the substrates.

e- **High-temperature tube furnace:** For heat treatment of deposited layers, a high-temperature tube furnace is used to control the temperature and annealing time of the materials.

f- **Metallization system:** For the manufacture of electrodes, a metallization system is used to deposit metallic contacts on the active layers of the solar cell.

g- **Optical or scanning electron microscope (SEM):** To inspect the morphology and structure of the deposited layers, as well as to verify the integrity of the device, an optical microscope or SEM is used.

h- **UV-Vis spectrometer and X-ray photoelectron spectroscopy (XPS):** To characterize the optical and electronic properties of the materials used, as well as the composition of the deposited layers, UV-Vis and XPS spectrometers are often used.

i- **Simulated solar light source:** To test the electrical performance of solar cell prototypes, a simulated solar light source is used to replicate solar irradiance conditions.

j- **Electrical measurement system** : To characterize the electrical performance of solar cells, an electrical measurement system is used to measure the currents and voltages generated under different illumination and polarization conditions.[28][29]

7- Advantages and Limitations for perovskite solar cells:

a- Advantages of perovskite solar cells:

- ***High Efficiency*****:** Perovskite solar cells have shown remarkable energy conversion efficiencies, often rivaling traditional solar technologies such as silicon. Their ability to effectively absorb sunlight over a wide range of wavelengths contributes to this high efficiency.
- ***Low manufacturing cost:*** The materials used in perovskites are relatively inexpensive, and their manufacturing process is less complex than that of traditional solar cells. This suggests potential for reducing production costs and expanding the accessibility of solar energy.
- ***Flexibility in design:*** Perovskites can be fabricated as thin films, making them suitable for a variety of applications, including curved and flexible surfaces. This flexibility opens the door to innovations in the design of solar devices and infrastructure.
- ***Potential for continuous improvement:*** Research into perovskite solar cells is very active, suggesting potential for continued performance improvement. Progress is being made regularly to address stability and durability issues, which could expand their range of applications.

b- Limitations of perovskite solar cells:

- ***Long-term stability:*** Perovskites are often subject to degradation, particularly in the presence of humidity, heat, or intense light. This instability limits their long-term durability and makes it necessary to develop protection and stabilization methods.

- ***Material Toxicity:*** Certain compounds used in perovskites, such as lead, raise environmental and health concerns. Proper management of these materials throughout the cell life cycle is therefore crucial to avoid potential risks.
- ***Performance Reproducibility*:** Achieving consistent and repeatable performance from a perovskite solar cell can be difficult due to the sensitivity of the materials to manufacturing and environmental conditions. This can lead to variations in cell-to-cell performance, posing challenges for large-scale industrialization.
- ***Production Scalability*:** Moving from laboratory manufacturing to large-scale production while maintaining high performance and low costs remains a challenge. Investments in research and development are necessary to overcome the technological and economic barriers associated with production scalability.

In short, although perovskite solar cells offer great potential to improve the efficiency and reduce costs of solar energy, challenges remain in terms of stability, material toxicity, performance reproducibility and scalability of production. These challenges require continued attention from researchers and industry for perovskites to become a competitive large-scale solar technology.[30][31]

8- Research and development :

a- **Recent advances** :

- Significant progress has been made in improving the efficiency of perovskite solar cells, with efficiencies regularly exceeding 25%.
- Research has also focused on increasing the long-term stability of perovskites, developing strategies to counteract degradation due to environmental factors.
- Significant efforts have been made to develop large-scale production methods, aimed at making commercial production of perovskite solar cells viable.

b- **Technological challenges** :

- Long-term stability remains a major challenge for perovskite solar cells, with rapid degradation under real-world environmental conditions.
- The toxicity of materials, particularly lead, raises environmental and health concerns, requiring less toxic alternatives.

- Ensuring reproducibility of perovskite solar cell performance remains a challenge, with significant variations observed between different manufacturing batches.

c- **Future areas for improvement** :

- The development of alternative perovskite materials that are less toxic and more stable could improve sustainability and environmental acceptability.
- Optimizing the interfaces and architectures of perovskite solar cells could lead to significant gains in efficiency and stability.
- The integration of perovskite solar cells with other solar technologies, such as silicon, provides opportunities to improve performance and overall reliability.

In summary, despite the progress made, technological challenges remain, but promising avenues for improvement are being explored to overcome these obstacles and fully exploit the potential of perovskite solar cells in the field of solar energy.[32]

9- Detailed comparison between an ordinary solar cell and a perovskite one:

a- Active material :

- ***Ordinary solar cell :*** Traditional solar cells generally use crystalline silicon as the active material. Silicon is abundant and well controlled in the photovoltaic industry.
- ***Perovskite Solar Cell :*** Perovskite solar cells use perovskite structural materials as the active material. These materials are often composed of mixtures of metal ions and halogenated anions, providing an efficient crystal structure for converting light into electricity.

b- Conversion efficiency :

- ***Ordinary solar cell :*** Silicon solar cells can achieve average efficiencies ranging from 15 to 22%, although high-efficiency cells can exceed these values.
- ***Perovskite Solar Cell :*** Perovskite solar cells have demonstrated higher conversion efficiency potential, often exceeding 25%. However, the long-term stability of these higher yields is still being developed.

c- Manufacturing cost :

- ***Ordinary solar cell :*** The manufacturing of silicon solar cells benefits from decades of research and development, which has significantly reduced manufacturing costs.
- ***Perovskite solar cell:*** Perovskite solar cells can be made from less expensive materials and with less complex manufacturing processes. This opens up the possibility of reducing production costs, but the technology still requires scaling to be fully competitive in the market.

d- Stability and durability :

- ***Ordinary Solar Cell :*** Silicon solar cells are known for their long-term stability and durability, with little performance degradation over time.
- ***Perovskite Solar Cell :*** Historically, perovskite solar cells have faced long-term stability issues, particularly regarding their sensitivity to humidity and light. However, intensive research is underway to improve the stability and durability of perovskite solar cells.

In conclusion, although perovskite solar cells offer the potential for higher conversion efficiency and potentially lower manufacturing costs, they still face challenges in long-term stability and durability to be fully competitive on the market.[33]

Conclusion :

This chapter took us to the heart of innovation with perovskite-based solar cells. We've explored every aspect of this emerging technology in detail, from the materials themselves to their potential applications in solar energy.

Going back in time, we discovered the fascinating history of perovskites, from their discovery to their current use in solar cells. Each stage of their evolution has been marked by significant breakthroughs and discoveries.

By examining how perovskite solar cells work, we have understood how these devices efficiently convert sunlight into electricity, paving the way for innovative applications in renewable energy.

We also explored the challenges and opportunities associated with the manufacturing and architecture of perovskite solar cells, as well as ongoing research to improve this promising technology.

Finally, we compared perovskite solar cells with traditional technologies, highlighting the advantages and limitations of each. This comparison gave us insight into the potential implications of perovskite solar cells for the future of solar energy.

In conclusion, this chapter has offered us a concise but comprehensive overview of perovskite-based solar cells, inviting us to envision a future where this innovative technology could play a key role in our quest for clean and sustainable energy.

CHAPTER FOUR

SIMULATION AND OPTIMIZATION OF MATERIAL-BASED SOLAR CELLS PEROVSKITES

Introduction:

Solar energy holds tremendous promise as a clean, renewable, and abundant source of power. However, realizing its full potential requires overcoming various technical challenges, particularly in the realm of solar cell technology. Our research focuses on a critical aspect of this technology, improving the efficiency of perovskite solar cells.

Perovskite solar cells have emerged as one of the most promising next-generation photovoltaic technologies due to their high efficiency potential, low-cost fabrication, and versatility in design. However, despite rapid advancements in recent years, there are still key hurdles to overcome, particularly in maximizing their efficacity and stability for practical applications.

One of the key determinants of a solar cell's efficiency is the Electron Transport Layer (ETL). This layer plays a crucial role in facilitating the efficient extraction and transport of photo-generated electrons from the light-absorbing layer to the external circuit. By optimizing the ETL, we can significantly enhance the overall performance of the solar cell.

The choice of materials for the ETL is paramount. In our study, we are exploring hybrid ETLs composed of combinations such as PBCM-SnS2, TiO2-SnO2, and PCBM-PCPB. These hybrid materials offer the potential to leverage the unique properties of each component to improve charge transport and collection efficiency, thereby boosting the overall performance of the solar cell.

By focusing on hybrid ETLs, we are not only aiming to enhance the potency of perovskite solar cells but also addressing broader challenges facing renewable energy adoption.

With SCAPS, we generate detailed graphs illustrating how each hybrid ETL behaves under different conditions. Additionally, we calculate current-voltage (J-V) characteristics, allowing us to determine key parameters such as short-circuit current density (Jsc), open-circuit voltage (Voc), form factor (FF), and efficiency (η).

In addition to these critical data points, SCAPS provides us with supplementary information such as external quantum efficiency (EQE), electric current density (I(V)), voltage power (P(V)), and energy band diagrams. These insights help us better understand the operation of perovskite solar cells and identify optimal configurations to enhance their performance.[34] [35]

1- SCAPS software

The SCAPS (Solar Cell Capacitance Simulator) software, designed by the team at Ghent University in Belgium, is an essential tool for professionals and researchers in the field of solar energy. This solar cell simulator can accurately evaluate the performance of photovoltaic devices, providing a robust platform for modeling and analysis of solar cell technologies in various configurations. Using SCAPS, it is possible to simulate complex structures of semiconductor devices, such as thin-film and hetero junction solar cells.

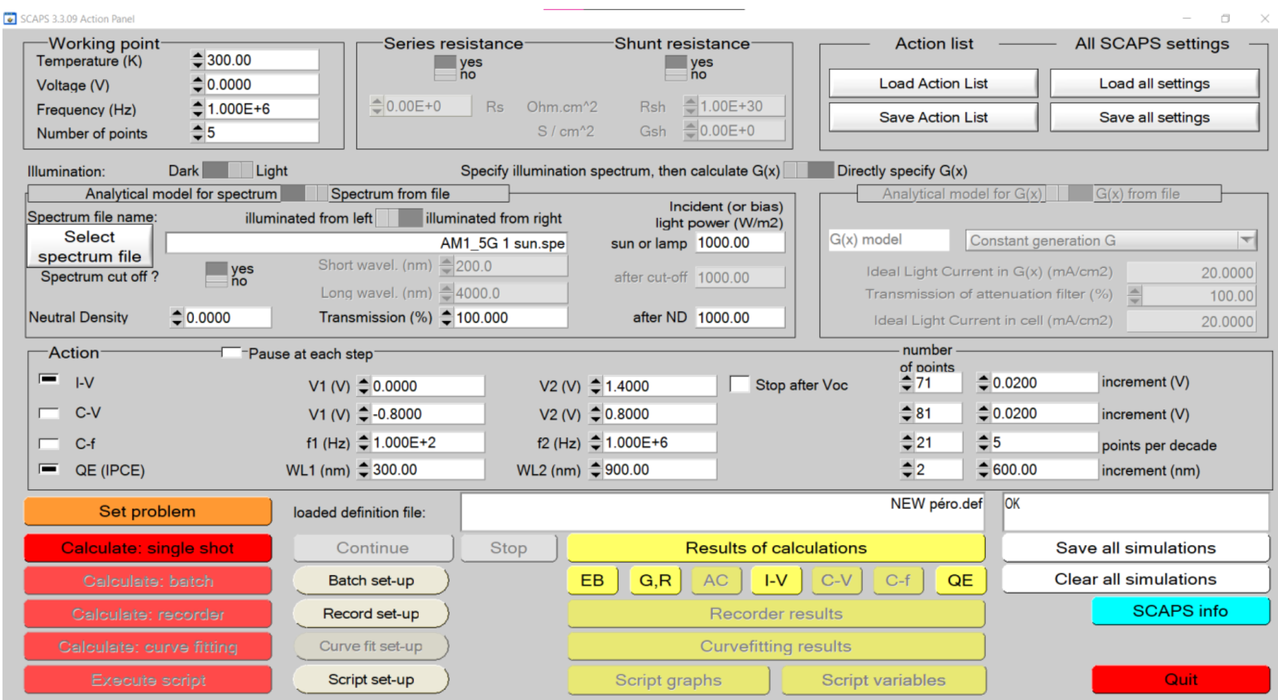


FIGURE 3.1: Main screen of SCAPS Softwar

The software provides detailed simulation of electrical characteristics such as Current-voltage (I-V) and capacitance-voltage (C-V) curves, while allowing analysis of the effects of environmental variables such as temperature and illumination on device performance. SCAPS' intuitive user interface is designed to facilitate complex simulations and interpretation of results, making this software accessible to PV experts and novices alike. [36] [37]

SCAPS thus finds its application not only in the development of new photovoltaic technologies but also as an educational tool for teaching the principles of photovoltaic engineering. In the following sections.

a) We will explore the features, usage method and practical applications of SCAPS in detail, illustrating its indispensable role in the development and optimization of solar technologies:

Category	**Attributes**	**Detailed Insights**
Origin of Software	University of Ghent, Belgium	Developed to support advanced research in photovoltaic technologies
Modeling Capabilities	- Semiconductor devices - Thin-film and heterojunction solar cells	Enables detailed modeling of various types of solar cells incorporating different layers and materials.
Simulations Performed	- Electrical characteristics (I-V, C-V curves) - Spectral and environmental responses	Analyzes the electrical and optical performance of cells under varying conditions, including changes in illumination and temperature
User Interface	Graphical User Interface (GUI)	Simplifies the setup of simulations, modification of parameters, and real-time results visualization.
Usage Procedure	1. Download 2. Install 3. Configure devices 4. Run simulations 5. Analyze results	- Accessible via the university's website. - Primarily installed on Windows platforms. - Allows customized configurations to test different hypotheses. - Provides tools for detailed data analysis
Practical Applications	-Academic research - Industrial development - Education and training	- Crucial for developing new solar technologies. - Used for preliminary evaluation before production. - Utilized in university curricula to teach the fundamentals of photovoltaic technology

Table 3.1 : Comprehensive Overview of SCAPS : Features, Usage, and Applications

The SCAPS software database:

Basic equations:

To precisely model the electrical properties of solar cells, the SCAPS software numerically solves the basic semiconductor equations with the drift diffusion approximation. Fish equation The Poisson equation is used to describe the relationship between potential and space charges.

$$\frac{\partial\varphi}{\partial x} = q\varepsilon[n(x) - p(x) - N_D^+(x) + N_A^-(x) - p_t(x) + n_t(x)] \quad (1)$$

Where $\boldsymbol{\varphi}$ is the potential, **q** is the elementary charge, **ε** is the permittivity, **n** is the density of free electrons, **p** is the density of free holes, $\mathbf{N_d}$ is the donor-type doping density, $\mathbf{N_a}$ is the acceptor-type doping density, $\mathbf{p_t}$ is the density of hole traps and $_{\mathbf{nt}}$ is the density of electron traps.

Continuity equations:

These equations make it possible to simultaneously analyze the drift, diffusion, generation and recombination of carriers:

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla . J_n G - R_n \quad (2)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\nabla . J_p G - R_p \quad (3)$$

Where, Gn (Gp) is the rate of optical generation of electrons (holes), and Rn (Rp) is the rate of recombination of electrons (holes).

$\boldsymbol{J_n}, \boldsymbol{J_p}$ are the current densities of electrons and holes given by the transport equations:

$$J_n = -qn\mu_n\nabla\Psi + \mathrm{q}D_n\nabla n \quad (4)$$

$$J_p = -qp\mu_p\nabla\Psi + \mathrm{q}D_p\nabla p \quad (5)$$

Where q is the elementary charge, μn (p) is the mobility of electrons (holes), and Dn (p) is the diffusion coefficient of electrons (holes).

The diffusion length describes the carrier transport capacity in a solar cell device. It depends on the diffusion coefficient and the lifetime of the carriers. This is represented in the equations:

$$L_n = \sqrt{D_n\tau_n} \quad (6)$$

$$L_p = \sqrt{D_p\tau_p} \quad (7)$$

[38]

2- Optimization of the perovskite cell based on CH3NH3PbI3 "MAI" with a Hybrid ETLs:

2.1- Presentation of the solar cell based on "MAI" with a Hybrid ETLs:

Our work consists of simulating a perovskite solar cell based on CH3NH3PbI3. We will optimize its electrical and geometric parameters in order to design a cell with optimal electrical efficiency. The structure studied is a planar n-i-p structure where the CH3NH3PbI3 absorbent layer is inserted between an n-type hybrid ET layer constituted by the transparent conductive oxide FTO and a p-type HT layer. In a perovskite solar cell, the hybrid ET layer plays an important role in improving performance.[39]

2.2- Structur of the cell :

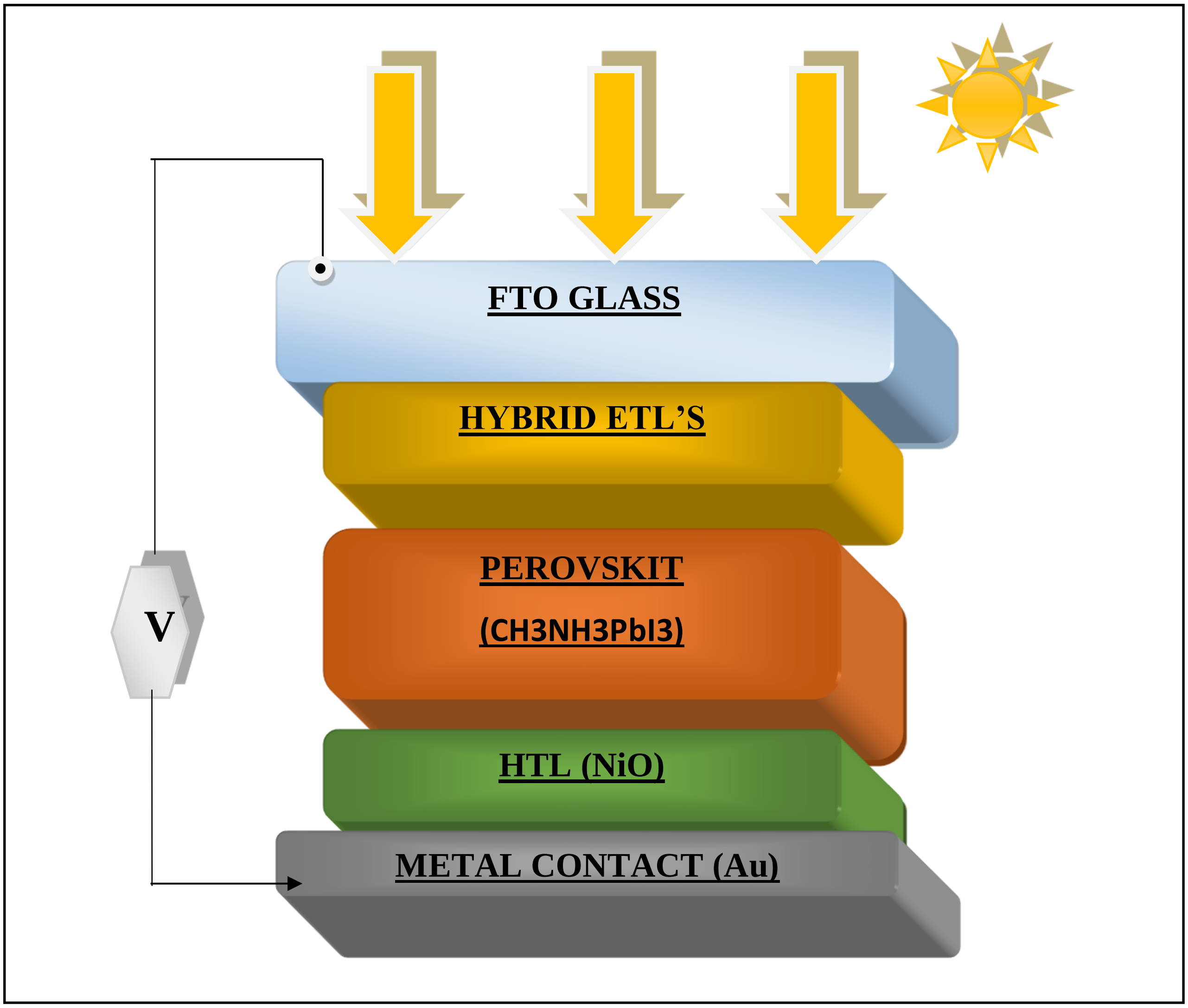


Figure 3.2: structure of our perovskite solar cell

The structure of this solar cell is composed of:

I - Hybrid Electron Transport Layer (ETL) :

I.I- PCBM-SnS2 : This combination offers synergy between PCBM, known for its electron acceptor properties, and SnS2, an emerging semiconductor material. PCBM promotes efficient charge separation at the interface with the perovskite layer, while SnS2 can act as an electron transport layer or buffer to reduce recombination losses and improve charge extraction. This marriage between a well-established electron acceptor and a promising semiconductor material opens prospects for more efficient and stable solar cells.

I.II- TiO2-SnO2 : The combination of TiO2 and SnO2 capitalizes on the advantages of each of these widely studied materials. TiO2 acts as an efficient electron transport layer due to its high electron mobility and favorable band alignment with the perovskite layer. On the other hand, SnO2 can be used to improve the quality of the interface between the perovskite layer and the electron transport layer, thereby reducing defects and improving charge collection efficiency. This combination contributes to the overall improvement of the performance of perovskite solar cells by optimizing electron extraction and interface quality.

I.III- PCBM-PCPB : The integration of PCBM with PCPB, a conjugated polymer specifically designed for organic photovoltaic applications, offers a complementary approach to improve the efficiency of perovskite solar cells. While PCBM acts as an electron acceptor, PCPB acts as a charge donor. The molecular design of PCPB is optimized to promote efficient exciton dissociation and charge transport within the active layer of the solar cell. This combination aims to achieve an optimal balance between charge transport and reduction of recombinations, thus leading to a significant improvement in device performance and stability.

Each of these hybrids represents an innovative approach to improving different aspects of perovskite solar cells, whether by optimizing charge separation, improving electron extraction, or promoting better interface quality. Continued research in this area is essential to fully exploit the potential of these emerging technologies and to advance towards more efficient and sustainable solar cells.

II - Perovskite Precursors « Methylammonium Lead Iodide (CH3NH3PbI3) » :

- Methylammonium lead iodide (CH3NH3PbI3) is a pivotal material extensively studied and applied in perovskite-based solar cells.
- As a hybrid organic-inorganic perovskite, it incorporates the organic methylammonium cation (MA) into the inorganic lead iodide (PbI3) lattice structure.
- This composition results in remarkable optoelectronic properties, including a high absorption coefficient, facilitating efficient light harvesting.
- Additionally, MAPbI3 perovskite exhibits a long carrier diffusion length, enhancing charge transport, and possesses a suitable bandgap for optimal energy conversion efficiency

III - Nickel Oxide (NiO) as Hole Transport Layer (HTL) :

- Nickel oxide (NiO) is a prominent choice for the Hole Transport Layer (HTL) in perovskite solar cells, offering several advantageous characteristics.
- Its energy levels align well with those of perovskite, facilitating efficient hole extraction and transport within the device.
- NiO demonstrates high transparency across the visible light spectrum, ensuring minimal light absorption and maximizing photon utilization.
- Moreover, its stability under ambient conditions contributes to the longevity and reliability of perovskite solar cell devices.

IV - FTO Glass :

Using FTO glass as a substrate for perovskite solar cells provides several benefits : high transparency, good electrical conductivity, compatibility with deposition processes, and stability. These key features promote efficiency and durability, driving forward the advancement of this innovative technology.

V- Metal contact (Au) :

Employing gold (Au) as a metal contact in perovskite solar cells brings several benefits. Gold boasts exceptional electrical conductivity, ensuring efficient charge extraction from the perovskite layer, thereby enhancing device performance. Moreover, its stability forms a robust interface with the perovskite, contributing to the overall longevity and reliability of the solar cell. [40] [41] [42][43]

2.3-Layer Energy Level (eV) :

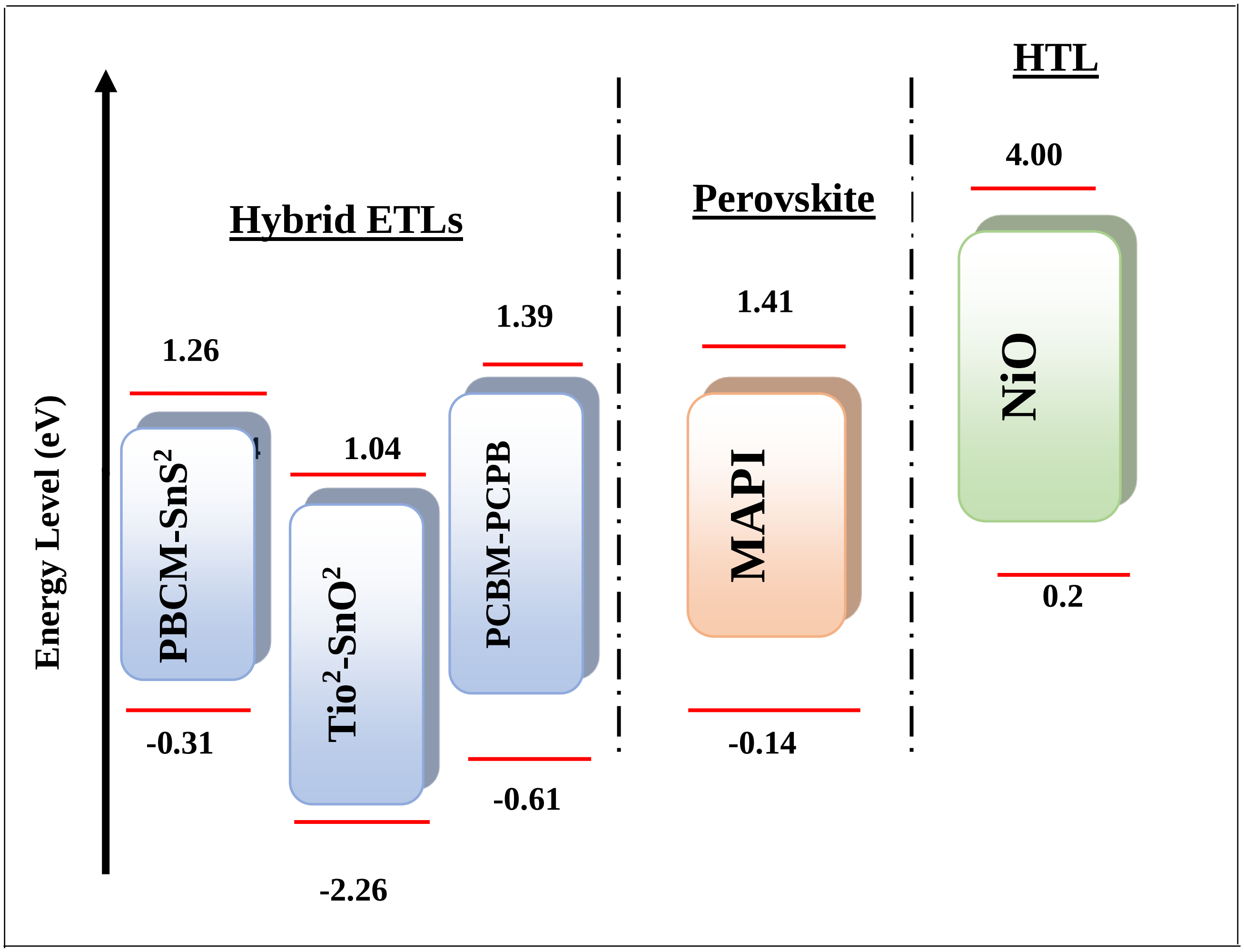


Figure 3.3 : Layer Energy Level (eV) [28] [29]

2.4- layer parameters used for simulation of perovskite solar cell:

Layer parameters	**Hybrid ETLs**			**Perovskite (MAI)**	**HTL (NiO)**
	PBCM-SnS^2	**Tio2-SnO2**	**PCBM-PCPB**		
Tickness (nm)	45	50	50	900	40
Band gap, E_g (eV)	1.57	3.3	2	1.55	3.8
Electron afnity, χ (eV)	4	4	3.9	3.9	1.46
Dielectric permittivity (relative), ε_r	4.2	9	3.9	30	10.7
CB efective density of states, NC ($1/cm^3$)	2.5×10^{19}	2.1×10^{18}	2.5×10^{21}	2×10^{18}	2.8×10^{18}
VB efective density of states, NV ($1/cm^3$)	2.5×10^{19}	1.8×10^{19}	2.5×10^{21}	2×10^{19}	1×10^{19}
Electron mobility, μ_n (cm^2/ V-s)	2.89×10^{-1}	30	5.5×10^{-4}	10	12
Hole mobility, μ_e (cm_2/ V-s)	2.89×10^{-1}	15	5.5×10^{-4}	10	2.8
Shallow uniform acceptor density, N_A ($1/cm^3$)	---------	---------	---------	1×10^{17}	1×10^{18}
Shallow uniform donor density, N_D ($1/cm^3$)	2.4×10^{17}	2×10^{20}	3×10^{17}	---------	---------
Total defect density, N_t ($1/cm^3$)	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{14}	1×10^{15}
Termal velocity of electrons and holes (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Capture cross section of electrons and holes (cm^2)	2×10^{-14}	2×10^{-14}	2×10^{-14}	2×10^{-14}	2×10^{-14}
Absorption coefcient, α (cm^{-1})	---------	---------	---------	1×10^{5}	---------

Table 3.2 : layer parameters used for simulation of perovskite solar cell. [30]

3-<u>Effect of the variation of the different hybrid electron transport layers on the characteristics of the cell :</u>

And these are Simulation results :

I - V_{OC} (Open circuit voltage) :

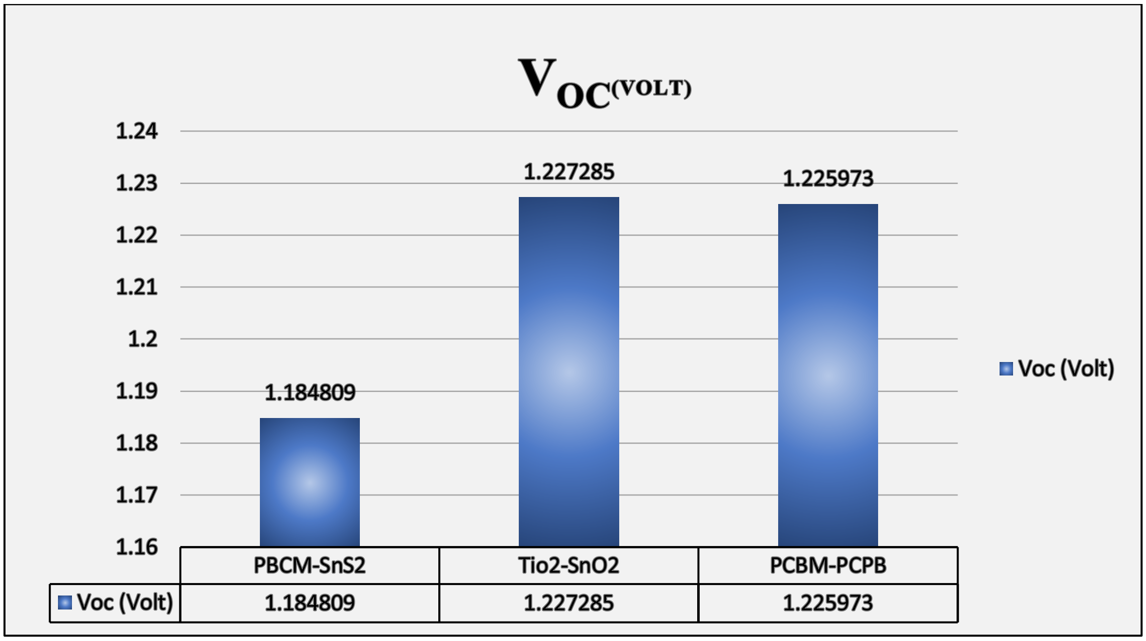


Figure 3.4 : Chart colomn of open cercuit voltage (Voc)

"This histogram represents the open-circuit voltages (VOC) of three different hybrid layers: PBCM-SnS2, Tio2-SnO2, and PCBM-PCPB. Each bar in the histogram corresponds to a specific voltage measured in volts. By analyzing the histogram, one can observe the VOC values for each hybrid layer. Trends or significant differences between the VOC voltages of the different layers could be investigated. For instance, one layer might exhibit a higher VOC voltage, indicating better performance or suitability under certain operating conditions. It would also be interesting to compare the distribution of VOC voltages between the different layers. A narrower distribution might suggest better uniformity or consistency of performance, while a wider distribution could indicate greater variability in sample properties or manufacturing processes."

II - J_{SC} (Short-circuit current density) :

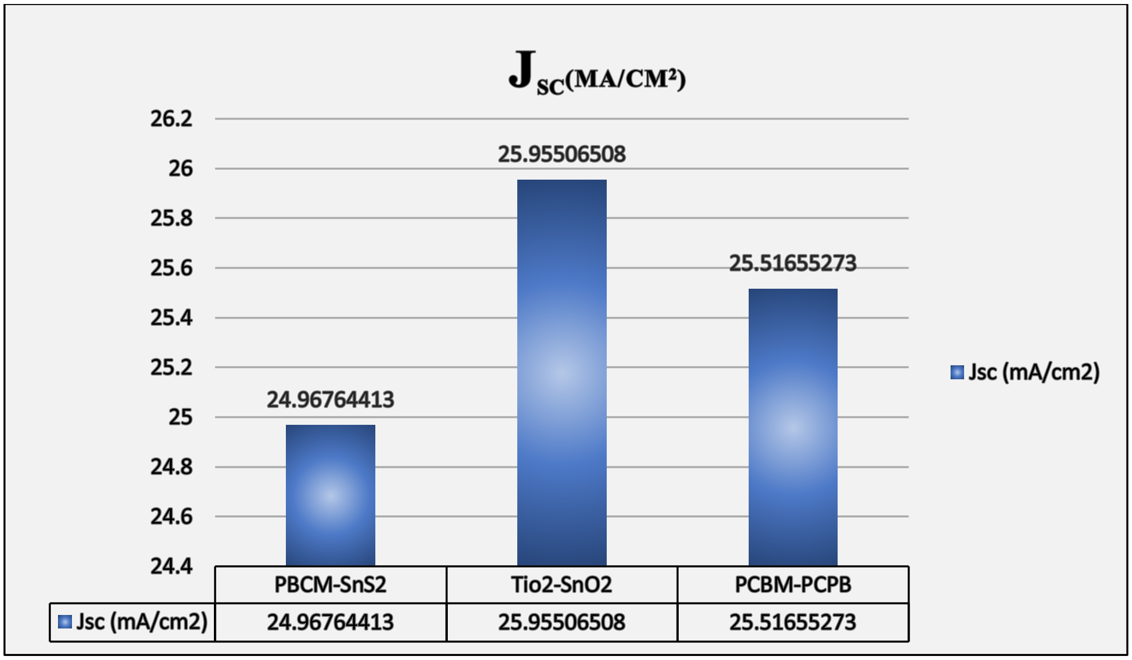


Figure 3.5 : Chart colomn of short-circuit current density (Jsc)

"This histogram represents the short-circuit current densities (JSC) of three different hybrid layers: PBCM-SnS2, Tio2-SnO2, and PCBM-PCPB. Each bar in the histogram corresponds to a specific current density measured in milliamperes per square centimeter (mA/cm2). By examining the histogram, one can observe the JSC values for each hybrid layer. This allows for the comparison of the short-circuit current densities between the different layers. We can look for trends or notable differences in the JSC values, which could indicate variations in the performance or characteristics of the hybrid layers. Additionally, analyzing the distribution of JSC values within each layer could provide insights into the consistency or variability of their performance. A narrower distribution might suggest more uniform characteristics across samples or batches, while a wider distribution could indicate greater variability."

III - FF (Form factor) :

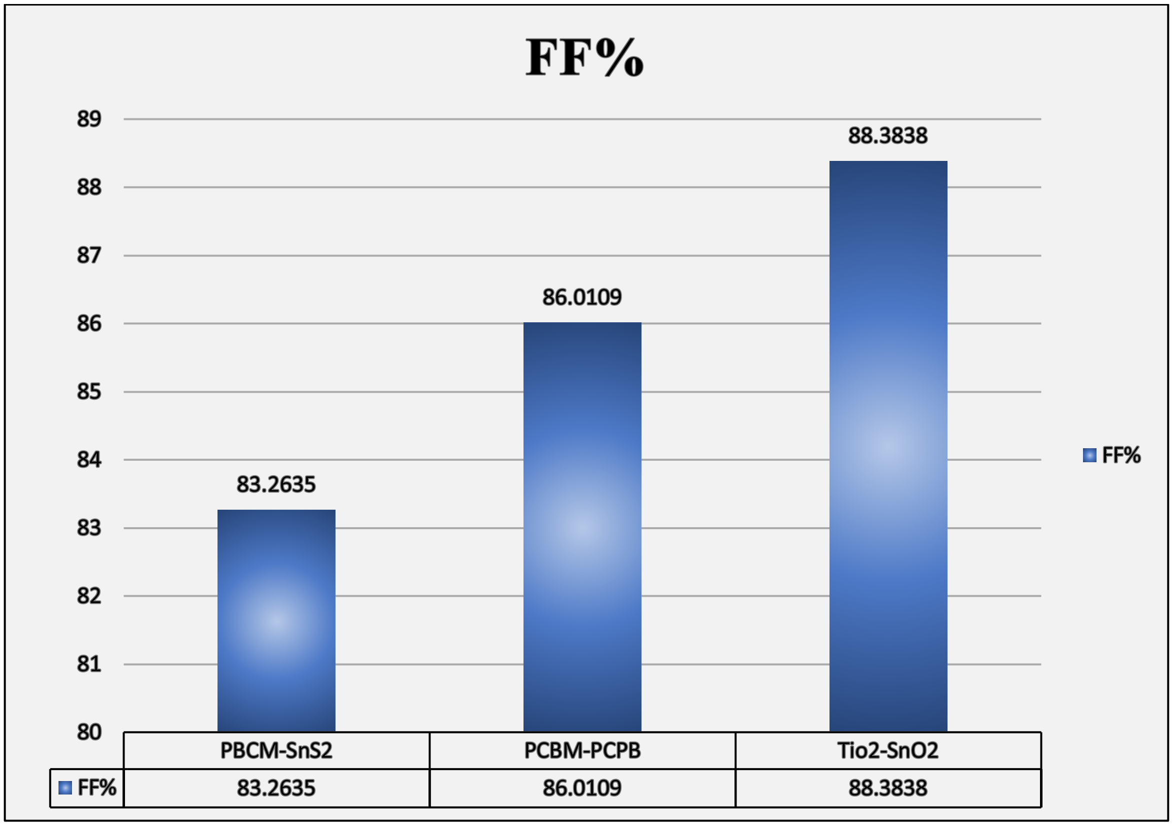


Figure 3.6 : Chart colomn of factor form (ff)

"Based on the provided data, it seems there might be a slight inconsistency or missing value for the Tio2-SnO2 layer. Assuming the stated value of 88.3838% , here's a comment on the histogram :

This histogram displays the form factor (FF) percentages of three distinct hybrid layers : PBCM-SnS2, Tio2-SnO2, and PCBM-PCPB. Each bar corresponds to the FF percentage of a particular layer.The form factor is a critical metric in assessing the efficiency of photovoltaic devices, indicating how effectively they convert incident sunlight into usable electrical power. Higher FF percentages typically denote more efficient conversion processes.Upon examining the histogram, we can compare the FF percentages among the different hybrid layers. Significant disparities in FF percentages may suggest variations in the efficiency of the devices within each layer.Moreover, analyzing the distribution of FF percentages within each layer can offer insights into the uniformity or variability of device performance. A narrower distribution indicates more consistent performance, while a wider distribution implies greater variability. "

IV - eTA (Efficiency) :

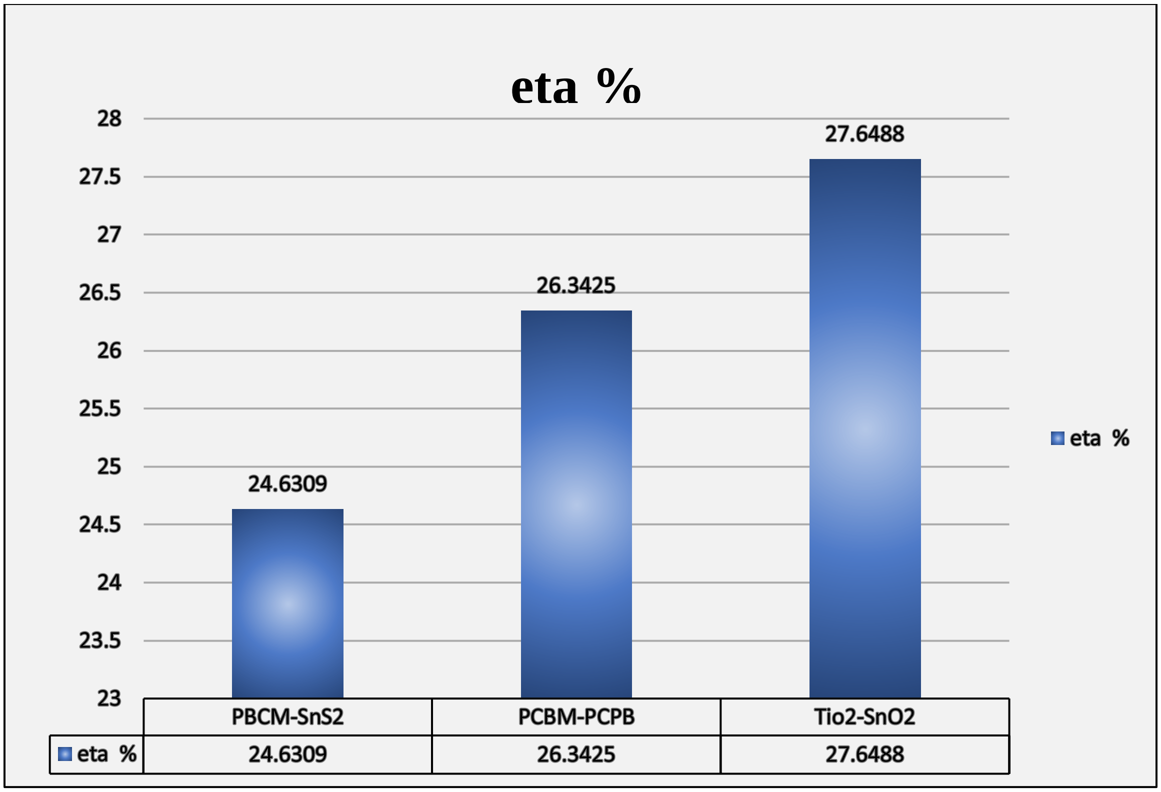


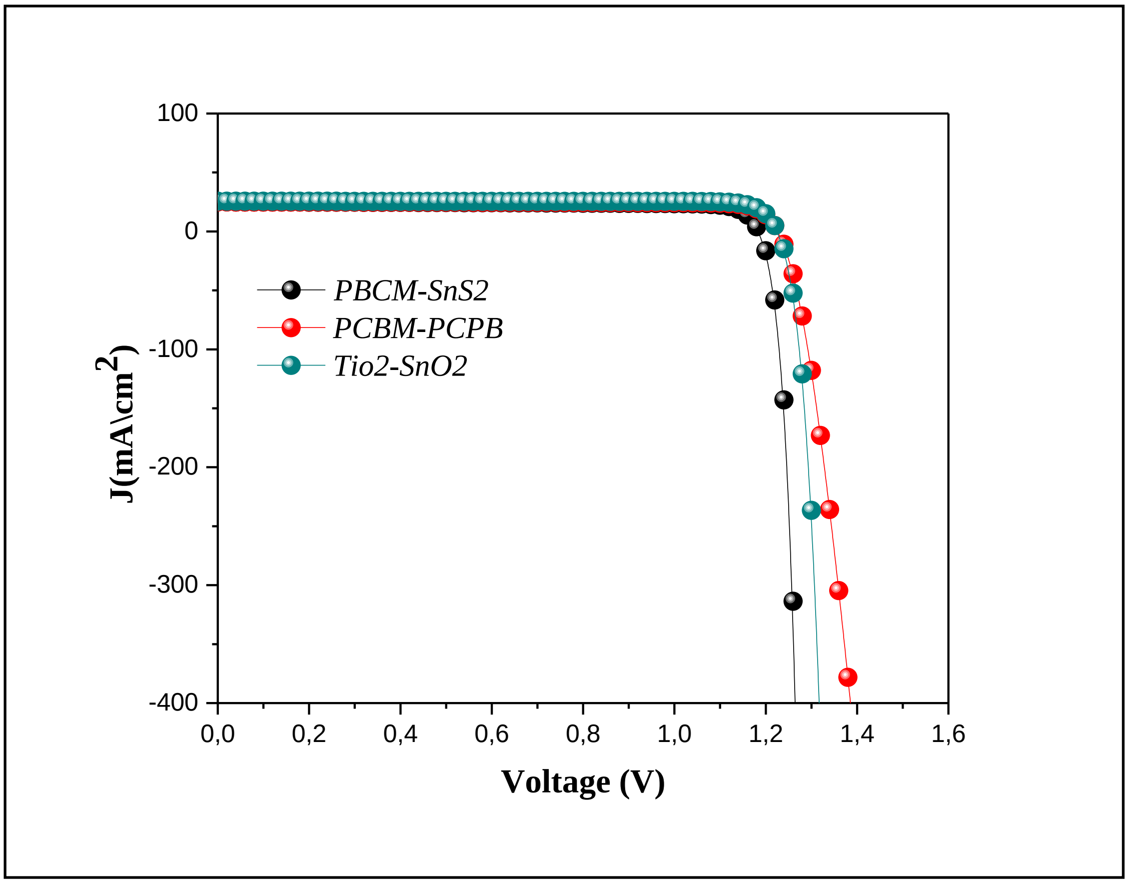
Figure 3.7 : Chart colomn of effciency (eTA)

"The histogram presents the efficiencies of three hybrid electron-transport layer configurations for solar cells, based on comparative data analysis. Among the three evaluated configurations, the TiO2-SnO2 hybrid electron transport layer stands out significantly with an estimated yield of 27.6477%. This observation suggests that the combination of TiO2-SnO2 offers better performance than the other configurations tested. These results highlight the critical importance of the choice of electron-transport layer configuration in the design of efficient solar cells. They also provide valuable insights for the future optimization of photovoltaic technologies." [30] [31]

Our results are validated by the study conducted by Sharma, H., Verma, V. K., Singh, R. C., Singh, P. K., and Basak, A. They performed a numerical analysis of high-efficiency CH3NH3PbI3 perovskite solar cells utilizing PEDOT : PSS as the hole transport material using the SCAPS 1D simulator. Their research, published in the Journal of Electronic Materials, confirms the high efficiency and performance metrics observed in our study (Sharma et al. 2023).

V - J(V) current voltage curves :

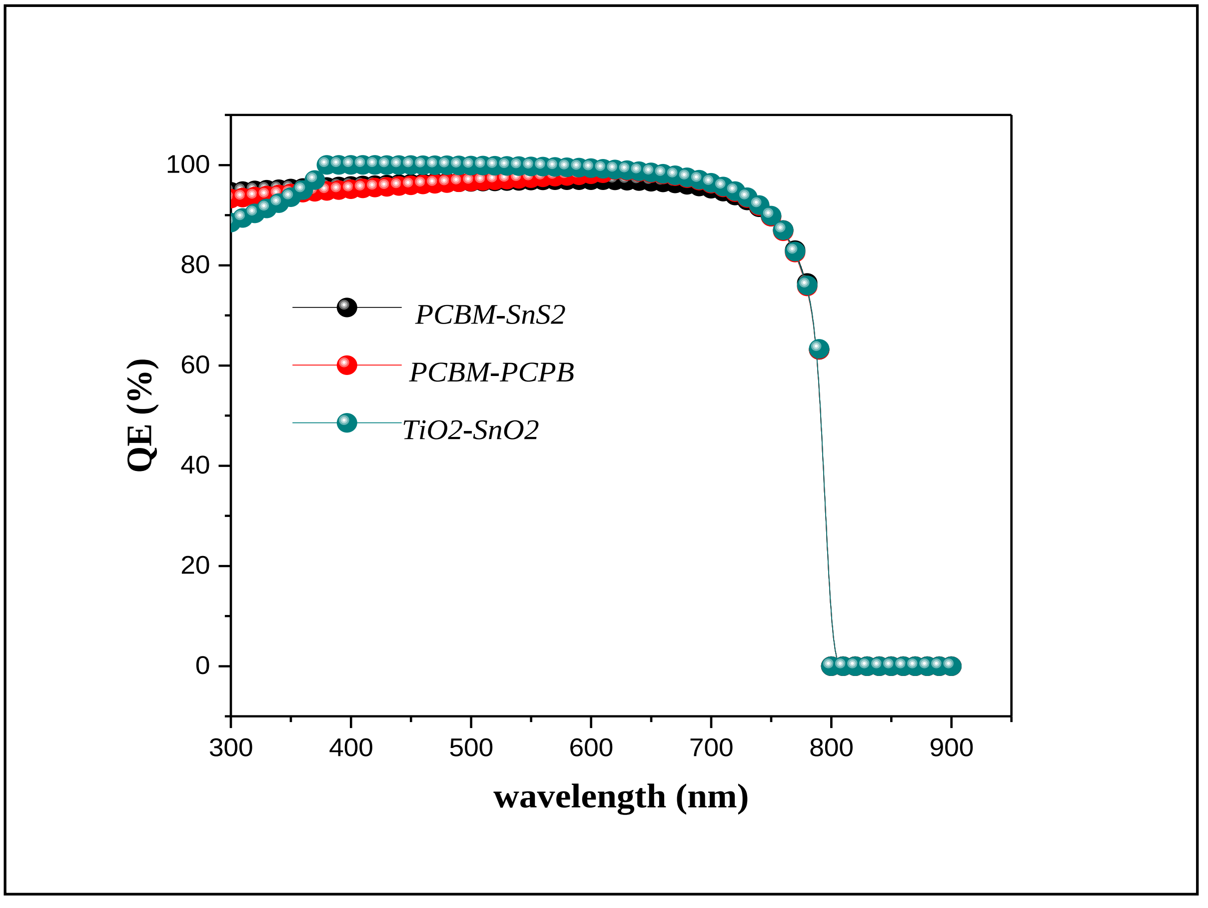
Evaluating the current-voltage (IV) characteristics of perovskite-based solar cells is essential for performance assessment, efficiency optimization, quality control, characterization of device degradation, and comparison with theoretical models. It provides critical data for determining key parameters, optimizing device components, ensuring reliability, understanding degradation mechanisms, and advancing perovskite photovoltaic technology.



After graphical analysis, although TiO^2-SnO^2 is not the highest curve over the entire voltage range, it demonstrates superior performance to PCBM-SnS^2 and PCBM-PCPB over part of the voltage range. This feature is crucial because it suggests that TiO^2-SnO^2 offers a compromise between the performance of the other two electronic hybrids, thus placing it as a strong and balanced option.[44] [45]

VI – (EQE) Quantum effeciency :

The quantum efficiency (EQE) of a solar cell measures its effectiveness in converting light into electricity by assessing the proportion of incident photons converted into free electrons. Its importance lies in evaluating performance under different lighting conditions, optimizing design for various wavelengths, guiding material selection for maximum light response, monitoring stability and degradation over time, and comparing performance with other solar technologies. In essence, QE is vital for maximizing solar cell efficiency, reliability, and competitiveness in the market.



The quantum efficiency (QE) curve presents the performance of the three ET layers (PBCM-SnS2, PCBM-PCPB and TiO2-SnO2) of the perovskite solar cell, as a function of wavelength. Among the three, the TiO2-SnO2 layer clearly stands out, with higher QE over a wide wavelength range. This observation suggests that the TiO2-SnO2 layer exhibits more efficient light absorption in the visible spectrum, which contributes to more efficient conversion of light to electricity. On the other hand, the curves corresponding to the PBCM-SnS2 and PCBM-PCPB layers present lower and less marked QEs, indicating less efficient light absorption. These results highlight the importance of the TiO2-SnO2 layer in optimizing the performance of the perovskite solar cell, thanks to its superior light absorption and electricity conversion efficiency.[33][35]

4- Final Design of a Perovskite Solar Cell Showing a Record Efficiency of 27.65% :

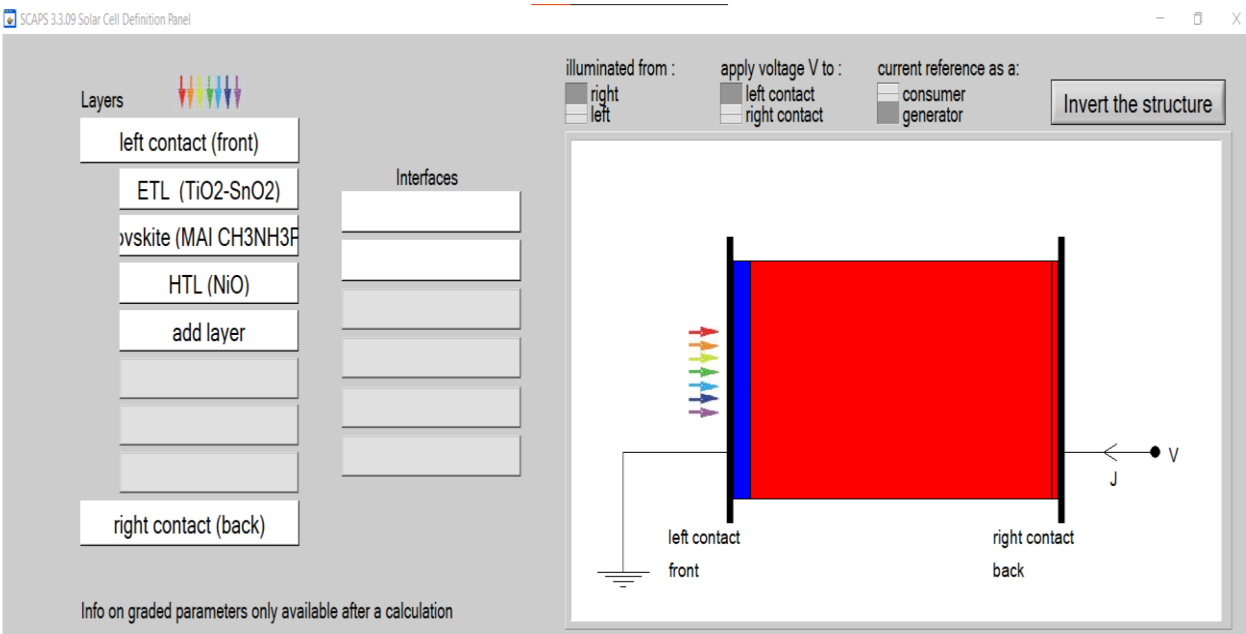


Figure 3.10: Screenshot taken from scaps software of the final structure of the cell

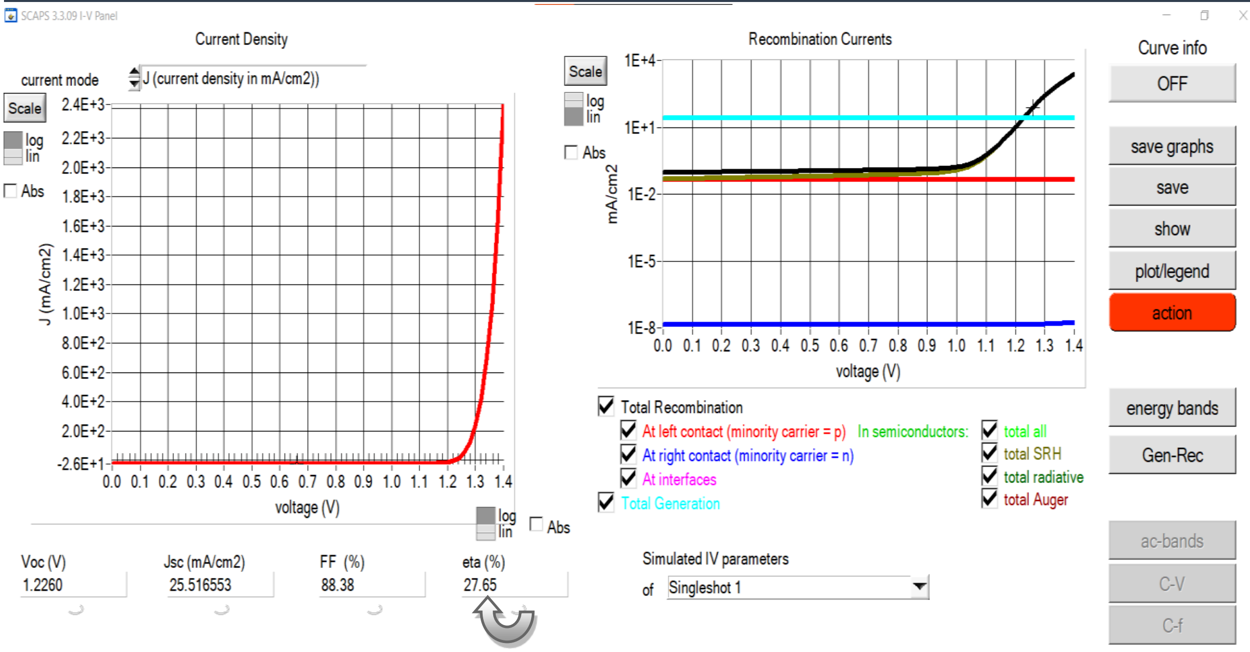


Figure 3.11: Screenshot taken with SCAPS software showing a record yield of 27.65%

Conclusion:

Our research highlights the critical importance of the Electron Transport Layer (ETL) in improving the efficiency and stability of perovskite solar cells. By focusing on hybrid ETLs like PBCM-SnS2, TiO2-SnO2, and PCBM-PCPB, we aim to enhance charge transport and collection efficiency, which are essential for optimal solar cell performance.

Using SCAPS simulations, we have identified key parameters and configurations that boost performance, providing insights into the behavior of hybrid ETLs under various conditions. These advancements are crucial for making perovskite solar cells more commercially viable and supporting broader renewable energy adoption.

In conclusion, optimizing the ETL is fundamental to advancing perovskite solar technology. This focus not only improves efficiency and stability but also contributes to global efforts in transitioning to clean and sustainable energy sources.

General Conclusion

This thesis explored the performance of perovskite solar cells through various simulations focused on the Electron Transport Layer (ETL) part of the solar cell structure, using the SCAPS software. This study distinguished itself by the innovation of using hybrid ETLs, combining different materials to optimize the performance of the solar cell.

The simulations demonstrated that using a hybrid ETL layer composed of TiO_2-SnO_2, combined with "MAI" as the absorber (perovskite) and nickel oxide as the HTL (Hole Transport Layer), achieved a record efficiency of 27.65%. These results are particularly significant as they demonstrate the potential of hybrid ETLs to improve the efficiency of perovskite solar cells.

The implications of this research are vast. On one hand, suggesting new design strategies for solar cells, aiming to combine different materials to maximize performance. On the other hand, it highlights the importance of optimizing the ETL layer in the overall efficiency of solar cells.

However, this study has certain limitations. The simulations, although indicative, require experimental validations to confirm the obtained results. Additionally, the long-term stability of solar cells with hybrid ETLs needs to be evaluated.

For future research, it would be pertinent to deepen experimental studies to validate the performance of hybrid ETLs under real conditions. Furthermore, exploring other material combinations for the ETL layers could lead to the discovery of even more efficient configurations. Finally, studying the stability and durability of perovskite-based solar cells with hybrid ETLs will be crucial for their commercialization.

In conclusion, this work has not only demonstrated the potential of hybrid ETLs to improve the performance of perovskite solar cells but has also provided a solid foundation for future research aimed at optimizing and stabilizing these devices. The perspectives opened by this study could significantly contribute to the advancement of solar technologies, offering more efficient and durable solutions for renewable energy production.

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