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### **Performance Comparison Between Two Perovskite Solar Cells Using SCAPS-1D Simulations**

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*To all of you, we express our deepest gratitude.*

# *Dedication*

*I dedicate this work to my beloved parents, whose love, support, and encouragement have been a constant source of strength throughout my journey.*

*To my brothers and sister, for always being there for me.*

*And all my friends and professors.*

*GHITRI Abdelhamid*

# *Dedication*

*I dedicate this dissertation*

*To my beloved parents, my mother and my father,  
for their patience, love, support, and constant  
encouragement.*

*To my family*

*I would also like to express my sincere gratitude to all my  
professors.*

***BOUZIANE Alaa-eddine***

## الملخص

يقدم هذا العمل دراسة عددية للخلايا الشمسية القائمة على مواد البيروفسكايت باستخدام برنامج SCAPS-1D ، مع التركيز على تأثير بنية الطبقة الماصة على أداء الجهاز. تمت دراسة بنيتين: بنية ذات طبقة ماصة واحدة قائمة على  $\text{MAPbI}_3$  ، وبنية ذات طبقتين ماصتين من  $\text{MAPbI}_3/\text{MASnI}_3$  ، ضمن تراكيب من نوع  $\text{FTO}/\text{WS}_2/\text{absorber}/\text{CuO}/\text{Au}$ . تم تحليل تأثير سمك الطبقة الماصة، وتركيز الشوائب القابلة، وكثافة العيوب، ودالة الشغل للقطب الخلفي بشكل منهجي على المعلمات الكهروضوئية. كما أُجريت مقارنة بين البنيتين من حيث نقل حوامل الشحنة، وجمع الشحنات، وكفاءة تحويل الطاقة الضوئية. وتوفر النتائج فهماً أفضل للعوامل الفيزيائية المتحكم في أداء الجهاز، وتساعد على تحديد الشروط المناسبة لتحسين أداء الخلايا الشمسية القائمة على البيروفسكايت ذات البنية ثنائية الطبقة.

## Abstract

This work presents a numerical study of perovskite solar cells based on SCAPS-1D, focusing on the effect of absorber architecture on device performance. Single-layer  $\text{MAPbI}_3$  and bilayer  $\text{MAPbI}_3/\text{MASnI}_3$  configurations are investigated using  $\text{FTO}/\text{WS}_2/\text{absorber}/\text{CuO}/\text{Au}$  structures. The influence of absorber thickness, acceptor concentration, defect density, and back-contact work function on the photovoltaic parameters is systematically analyzed. A comparative assessment of the single-layer and bilayer configurations is performed in terms of carrier transport, charge collection, and power conversion efficiency. The results provide a physical understanding of the parameters governing device performance and identify suitable conditions for the optimization of bilayer perovskite solar cells.

## Résumé

Ce travail présente une étude numérique de cellules solaires à base de pérovskites à l'aide du logiciel SCAPS-1D, portant sur l'influence de l'architecture de l'absorbeur sur les performances du dispositif. Deux configurations sont étudiées : une structure à couche absorbante unique à base de  $\text{MAPbI}_3$  et une structure à double couche  $\text{MAPbI}_3/\text{MASnI}_3$ , intégrées dans des architectures  $\text{FTO}/\text{WS}_2/\text{absorbeur}/\text{CuO}/\text{Au}$ . L'influence de l'épaisseur de l'absorbeur, de la concentration en accepteurs, de la densité des défauts et du travail de sortie du contact arrière sur les paramètres photovoltaïques est systématiquement analysée. Une comparaison des deux configurations est réalisée en termes de transport des porteurs, de collecte des charges et de rendement de conversion photovoltaïque. Les résultats permettent de mieux comprendre les paramètres physiques régissant les performances du dispositif et d'identifier des conditions appropriées pour l'optimisation des cellules solaires à pérovskite à double couche.



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# NOMENCLATURE

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# *Nomenclature*

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PV : Photovoltaic

PSC : Perovskite Solar Cell

SCAPS-1D : Solar Cell Capacitance Simulator in One Dimension

ETL : Electron Transport Layer

HTL : Hole Transport Layer

FTO : Fluorine-Doped Tin Oxide

WS<sub>2</sub> : Tungsten Disulfide

MAPbI<sub>3</sub> : Methylammonium Lead Iodide

MASnI<sub>3</sub> : Methylammonium Tin Iodide

CuO : Copper Oxide

Au : Gold

V<sub>oc</sub> : Open-Circuit Voltage

J<sub>sc</sub> : Short-Circuit Current Density

FF : Fill Factor

PCE : Power Conversion Efficiency

AM : Air Mass

AM0 : Air Mass 0

AM1.5D : Air Mass 1.5 Direct

AM1.5G : Air Mass 1.5 Global

$\theta_z$  : Zenith Angle

$\lambda$  : Wavelength

$\nu$  : Frequency

$c$  : Speed of Light

$h$  : Planck's Constant

$E$  : Photon Energy

$E_g$  : Band Gap Energy

$B_v$  : Valence Band

$B_c$  : Conduction Band

$E_D$  : Donor Energy Level

$E_A$  : Acceptor Energy Level

ZCE : Space Charge Zone

P-type : P-Type Semiconductor

N-type : N-Type Semiconductor

$I_{ph}$  : Photogenerated Current

$I_0$  : Incident Light Intensity

$I$  : Transmitted Light Intensity

$\alpha$  : Absorption Coefficient

$l$  : Material Thickness

$T$  : Transmittance / Temperature

$A$  : Absorbance

DO : Optical Density

$I_{0bsc}$  : Dark Current

$I_s$  : Diode Saturation Current

$D$  : Diffusion Coefficient

$L_d$  : Diffusion Length

$\tau$  : Carrier Lifetime

$e$  : Elementary Charge

$q$  : Elementary Charge

$K$  : Boltzmann Constant

$n_i$  : Intrinsic Carrier Concentration

$D_n$  : Electron Diffusion Coefficient

$D_p$  : Hole Diffusion Coefficient

$L_n$  : Electron Diffusion Length

$L_p$  : Hole Diffusion Length

$I$ – $V$  : Current–Voltage Characteristic

$P$ – $V$  : Power–Voltage Characteristic

$C$ – $V$  : Capacitance–Voltage Characteristic

$C$ – $f$  : Capacitance–Frequency Characteristic

$I_{s1}$  : Saturation Current of Diode  $D1$

$I_{s2}$  : Saturation Current of Diode  $D2$

$n_1$  : Ideality Factor of Diode  $D1$

$n_2$  : Ideality Factor of Diode  $D2$

$R_s$  : Series Resistance

$R_p$  : Parallel Resistance

$R_{sh}$  : Shunt Resistance

$I_{cc}$  : Short-Circuit Current

$V_{co}$  : Open-Circuit Voltage

$P_{max}$  : Maximum Power

$P_m$  : Maximum Power Point

$V_m$  : Maximum Voltage

$I_m$  : Maximum Current

$MPP$  : Maximum Power Point

$FF_0$  : Ideal Fill Factor

$r_s$  : Normalized Series Resistance

$\eta$  : Electrical Conversion Efficiency

$P_{in}$  : Input Power

$P_{out}$  : Output Power

$RS$  : Spectral Response

$RS(\lambda)$  : Spectral Response as a Function of Wavelength

$IQE$  : Internal Quantum Efficiency

$EQE$  : External Quantum Efficiency

$R(\lambda)$  : Reflection Coefficient

$SRH$  : Shockley–Read–Hall Recombination

$E_p$  : Recombination Center Energy Level

$E_c$  : Conduction Band Energy Level

$E_v$  : Valence Band Energy Level

$IPV$  : Impurity Photovoltaic Effect

$g(x)$  : Generation Rate as a Function of Position

$V$  : Voltage

$F$  : Frequency

$\chi$  : Electron Affinity

$\epsilon_r$  : Relative Dielectric Permittivity

$N_C$  : Effective Density of States in the Conduction Band

$N_V$  : Effective Density of States in the Valence Band

$\mu_n$  : Electron Mobility

$\mu_h$  : Hole Mobility

$N_A$  : Shallow Uniform Acceptor Density

$N_D$  : Shallow Uniform Donor Density

$N_t$  : Total Defect Density

$\sigma_e$  : Electron Capture Cross Section

$\sigma_h$  : Hole Capture Cross Section

$E_r$  : Defect Energy Level

$f$



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# GENERAL INTRODUCTION

The transition toward low-carbon energy systems has intensified research into photovoltaic (PV) technologies capable of converting solar radiation into electricity with high efficiency, low material consumption, and scalable manufacturing. Among emerging photovoltaic technologies, metal-halide perovskite solar cells (PSCs) have attracted exceptional attention because their optical and electronic properties can be tuned through composition and device engineering. Recent reviews emphasize that perovskite absorbers combine strong optical absorption, adjustable band gaps, favorable charge-transport characteristics, and compatibility with relatively simple thin-film processing, while continuing challenges concern operational stability, defects, environmental exposure, toxicity, and large-area manufacturing [1,3,10-12].

The rapid development of PSCs has also expanded the scope of photovoltaic research from conventional single-junction devices toward multijunction and tandem architectures. In a single-junction solar cell, the absorber band gap imposes a fundamental compromise between photocurrent generation and voltage. Tandem architectures address this limitation by combining absorbers with different band gaps so that different portions of the solar spectrum can be utilized more effectively. In particular, all-perovskite tandems can combine a wider-band-gap top absorber with a narrower-band-gap bottom absorber, providing a route toward higher theoretical and practical efficiencies [1,8]. Recent research on perovskite/silicon tandems similarly demonstrates the importance of complementary band gaps, optical management, interfacial charge extraction, and long-term stability [9].

## Motivation and Scientific Context

Despite their impressive photovoltaic potential, PSCs remain sensitive to a large number of interacting material and device parameters. The absorber thickness affects optical absorption and carrier collection; doping influences the internal electric field and charge extraction; bulk and interface defects provide recombination pathways; and the energy-level alignment between the absorber, electron transport layer (ETL), hole transport layer (HTL), and electrodes affects carrier selectivity and extraction. Consequently, optimizing one parameter independently may not identify the most favorable device operating point. Recent literature continues to identify defect-mediated non-radiative recombination, interface losses, instability,

and scale-up as central issues in translating high laboratory efficiencies into durable photovoltaic technology [3,8,10-11].

The choice of charge-transport layers is also important because they determine the direction and selectivity of photogenerated-carrier extraction. Modern perovskite devices employ a variety of ETLs and HTLs, and their performance depends not only on their intrinsic mobility and conductivity but also on band alignment, interfacial defect density, and chemical compatibility with the absorber. Recent advances in inverted architectures illustrate how transport-layer and interface engineering can simultaneously improve efficiency, operational reliability, and compatibility with tandem configurations [7].

## **Role of Numerical Modelling in Photovoltaic Design**

Experimental optimization of photovoltaic devices can require a large number of fabrication and characterization cycles because several parameters are coupled. Numerical device simulation therefore provides a complementary approach for examining the influence of material properties and device architecture before experimental implementation. In particular, the Solar Cell Capacitance Simulator (SCAPS-1D) is widely used to model one-dimensional semiconductor devices and to evaluate the influence of layer thickness, carrier concentrations, defect states, interface properties, temperature, and contact conditions on photovoltaic output. Recent studies have applied SCAPS-1D to conventional and lead-free perovskite devices, including investigations combining numerical simulation with first-principles calculations [4-6].

The physical basis of the numerical analysis is the self-consistent solution of semiconductor transport equations. The electrostatic potential is obtained from Poisson's equation, while carrier distributions are determined through the continuity equations for electrons and holes. Together with the constitutive relations for drift and diffusion currents and the selected recombination and generation models, these equations provide the spatial distributions required to calculate current-density-voltage characteristics and photovoltaic parameters. This modelling framework makes it possible to establish relationships between microscopic or layer-level parameters and macroscopic indicators such as open-circuit voltage ( $V_{oc}$ ), short-circuit current density ( $J_{sc}$ ), fill factor (FF), and power-conversion efficiency

(PCE). Recent SCAPS-1D studies demonstrate the usefulness of this approach for identifying favorable thicknesses, defect densities, transport-layer properties, and energy-level configurations [4-6].

## **Research Problem and Objectives**

Within this context, the present thesis focuses on the numerical investigation and optimization of perovskite solar-cell structures. The work considers both a single-absorber configuration and a bilayer absorber configuration, with particular attention to MAPbI<sub>3</sub>-based devices and the incorporation of MASnI<sub>3</sub> as a narrower-band-gap absorber. The selected structures use FTO as the transparent conducting substrate, WS<sub>2</sub> as the electron transport layer, CuO as the hole transport layer, and Au as the rear contact. The study therefore combines material selection, energy-level alignment, semiconductor device modelling, and systematic parameter optimization.

The principal objectives are: (i) to introduce the physical principles governing photovoltaic energy conversion and the operation of solar-cell devices; (ii) to establish the numerical methodology used for one-dimensional device simulation; (iii) to investigate the influence of absorber thickness, shallow acceptor concentration, defect-trap density, and back-contact work function on device performance; (iv) to compare single-layer and bilayer absorber architectures; and (v) to identify parameter combinations that provide improved carrier collection and photovoltaic conversion while clarifying the physical mechanisms responsible for performance changes.

## **Organization of the Thesis**

The thesis is organized into three main chapters. Chapter I presents general information on solar cells, including the fundamental principles of photovoltaic conversion, the main characteristics of solar-cell technologies, and the physical parameters used to evaluate photovoltaic performance. Particular attention is given to the operating principles relevant to perovskite solar cells and to the role of the different functional layers in a photovoltaic device.

Chapter II describes the numerical simulation methodology based on SCAPS-1D. The chapter introduces the physical equations used in the simulation, the material and interface parameters

required to construct the device, the boundary conditions and illumination conditions, and the photovoltaic quantities extracted from the calculated current-density-voltage response. The chapter also establishes the numerical procedure used to evaluate the effect of the principal device parameters.

Chapter III presents the numerical optimization of single-layer and bilayer perovskite solar cells. As detailed in the present work, the analysis systematically varies absorber thickness, shallow acceptor density, defect-trap density, and back-contact work function. The bilayer architecture is examined as a means of extending spectral utilization through the combination of MAPbI<sub>3</sub> and MASnI<sub>3</sub>. The results are interpreted in terms of photocurrent generation, voltage generation, charge extraction, recombination, and the trade-offs associated with absorber thickness and electrical properties.

The thesis combines the general principles of photovoltaic devices with one-dimensional numerical modelling to establish a systematic framework for understanding and optimizing perovskite solar-cell architectures. The approach is particularly relevant to the current development of tandem photovoltaics, where improvements in efficiency must be considered together with defect control, interface engineering, operational stability, and scalability [1,8-12].

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## **I.1 Introduction:**

Solar photovoltaic energy refers to the generation of electricity from sunlight through the use of solar panels, where the solar cell acts as the main electronic component. Semiconductors are considered some of the most appropriate materials for photovoltaic applications. When sunlight photons hit the semiconductor material, they are absorbed and create electron-hole pairs, which participate in generating electric current.

In this chapter, we first introduce the basic concepts related to solar radiation, photovoltaic conversion, and the photoelectric effect. This background helps in understanding the principles that form the basis of the rest of the study. The second section is dedicated to the conventional solar cell, including its operating mechanism, current-voltage (I-V) characteristics, and the main parameters used to determine solar cell efficiency. In addition, several theoretical models related to photovoltaic cells will be discussed. Prior to that, the fundamental concepts of the PN junction, which is an essential part of solar cell operation, will also be presented.

## **I.2 Concept of Solar Radiation**

### **I.2.1 Solar Energy Source**

The sun releases a huge amount of energy, and taking advantage of this free resource is highly beneficial. Sunlight spans a broad range of wavelengths, starting from ultraviolet (UV) radiation (10–400 nm), passing through visible light (400–700 nm), and extending to infrared (IR) radiation (>700 nm) [1]. Since the highest irradiation intensity lies within the visible light region, solar cell designers should focus on materials that exhibit strong absorption in this part of the spectrum.

Solar irradiance changes according to variations in the sun's emitted energy, geographical location, time, and atmospheric conditions. Therefore, establishing standard testing and research conditions is necessary. For this purpose, the photovoltaic division of the American Society for Testing and Materials (ASTM) defined three standard test conditions based on different air masses (AM1.5G, AM1.5D, and AM0), as illustrated in Figure I.1.

The air mass (AM) concept represents the path length traveled by sunlight through the atmosphere before reaching the Earth's surface. It can be determined using the following equation [1]:

$$AM = \frac{1}{\cos(\theta_z)} \quad [I.1]$$

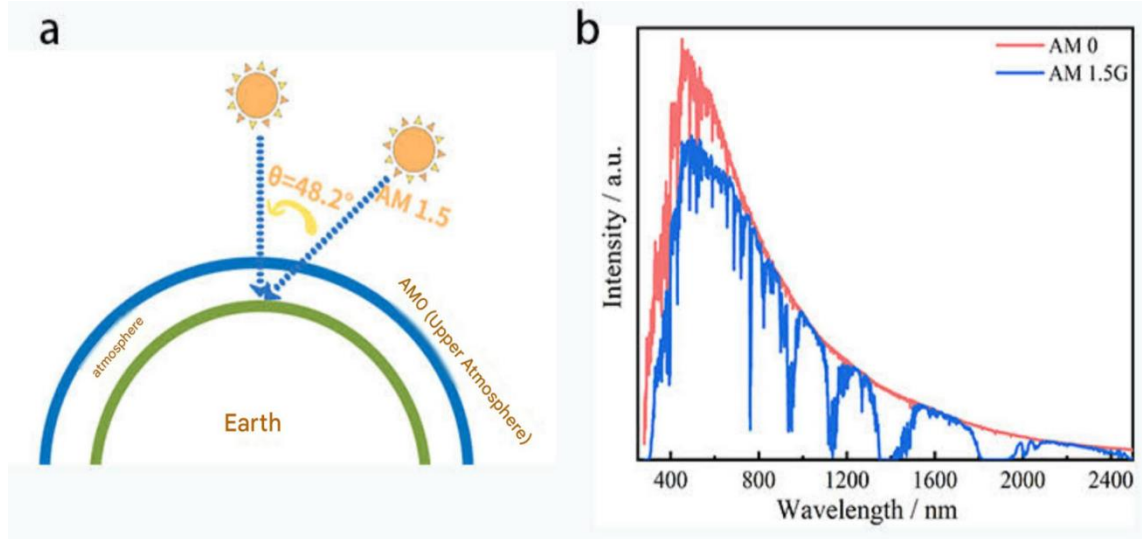


**Figure I.1** Understanding the Differences Between AM 0, AM 1.5, and AM 1.5G in the Solar Energy Field with a Single Article [6]

## I.2.2 Solar Spectrum

The solar spectrum is produced by the decomposition of light into its various wavelengths. It is composed of several colored radiations, each corresponding to a specific wavelength range [2].

The reconciliation between the two theories of light, namely the wave theory and the corpuscular theory, was achieved only in the 20th century through the discovery of the photon by Planck and Einstein. This became possible because light actually possesses a dual nature.

- Light behaves as an electromagnetic wave, meaning a periodic oscillation characterized by its wavelength  $\lambda$  or its frequency  $\nu$ . The higher the frequency, the shorter the wavelength, and vice versa, where  $c$  represents the speed of light.

$$\nu = \frac{c}{\lambda} \quad [I.2]$$

- It is also a beam of photons that is like "grains of light." carriers of an amount of energy, which depends on their wavelength, according to Louis' formula de Broglie:

$$E = h\nu = \frac{hc}{\lambda} \quad [I.3]$$

h: Plank's constant

Table.I.1 gives the characteristic energy values of photons for various wavelengths, as well as the areas corresponding to the light spectrum.

| Zone               | $\lambda$ ( $\mu\text{m}$ ) | $E_{\text{photon}}$ (eV) |
|--------------------|-----------------------------|--------------------------|
| Ultraviolet        | 0.2                         | 6.3                      |
| Visible Blue       | 0.4                         | 3.1                      |
| Visible Jaune Vert | 0.5                         | 2.48                     |
| Visible Rouge      | 0.78                        | 1.59                     |
| Infrarouge         | 1                           | 1.24                     |
| Infrarouge         | 2                           | 0.62                     |
| Infrarouge         | 4                           | 0.31                     |

**Table.I.1** Energy values of photons from the solar spectrum [2].

### I.2.3 Photovoltaic Effect

The photovoltaic effect is strongly related to the photoelectric effect, which was first discovered by Antoine Becquerel. During this experiment, an electric current was generated when two electrodes immersed in a fluid were exposed to light. This discovery, reported in 1839 by his son Edmond Becquerel, was only fully explained much later through the theories of Albert Einstein, who received the Nobel Prize in Physics in 1921 for this contribution [5].

A major advancement in photovoltaics occurred in 1954 when researchers at Bell Laboratories accidentally noticed that PN diodes generated a current when exposed to light [5]. A few months later, they introduced the first silicon solar cells, which achieved a conversion efficiency of nearly 6%. Since then, photovoltaic technology has progressed significantly and has become a dependable and long-lasting energy source [5].

More specifically, the photovoltaic effect is a physical phenomenon that takes place when electromagnetic radiation interacts with semiconductor materials, producing a small electric current in a semiconductor exposed to light, particularly sunlight [6], the Figure I.2 show a schematic explication of the photovoltaic effect.

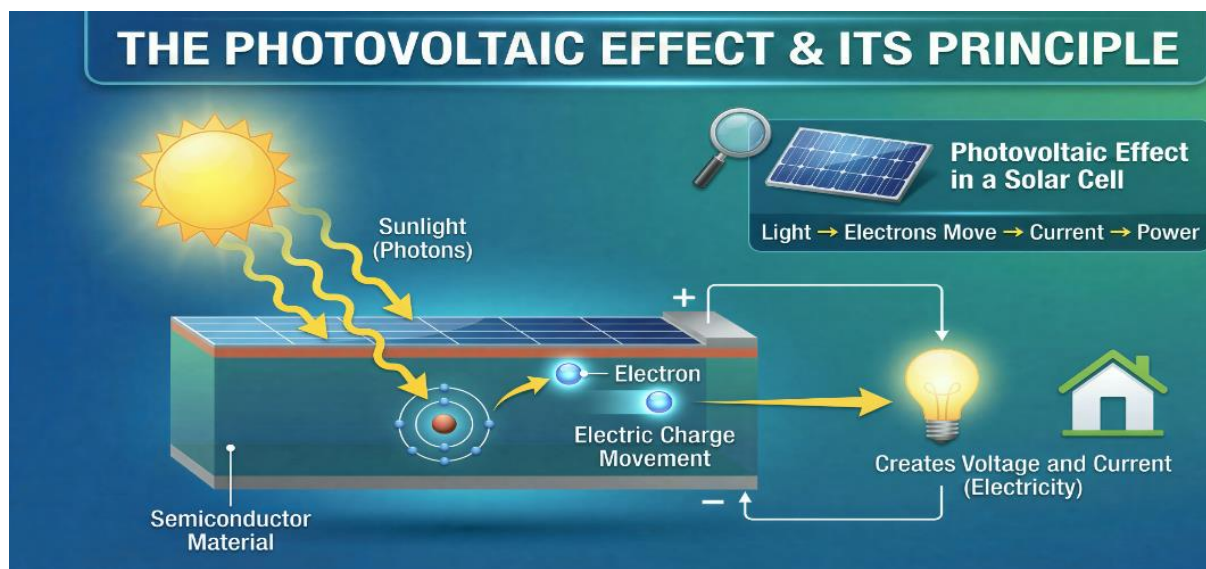


**Figure I.2** The photovoltaic effect

When a photon reaches a semiconductor material, two situations may occur. If the photon energy is lower than the semiconductor band gap energy ( $E_g$ ), the material remains transparent to the photon [6]. However, if the photon energy is equal to or greater than  $E_g$ , the photon is absorbed, leading to the creation of an electron-hole pair: an electron moves from the valence band ( $B_v$ ) to the conduction band ( $B_c$ ), leaving behind a hole in the valence band [6]. The separation and collection of this electron-hole pair before recombination make it possible to generate an electric current. This phenomenon forms the operating principle of many optoelectronic devices.

### I.3 Concept of a Solar Cell

The first solar cell was characterized by a simple structure; however, it was unable to provide high performance or satisfy the power demands of electrical loads. It also suffered from several major limitations, including considerable losses caused by reflection, ohmic contacts, and carrier recombination. Consequently, this configuration underwent multiple improvements.

The current optimized structure, designed to achieve better performance, is based on a multi-layer configuration that includes the PN junction, as shown in Figure I.3, which forms the core of the solar cell. This junction plays a key role in the generation and separation of charge carriers. Additional layers are incorporated around the p-n junction, including the window layer, the anti-reflection layer, the back surface field layer, and the metallic electrodes [7].

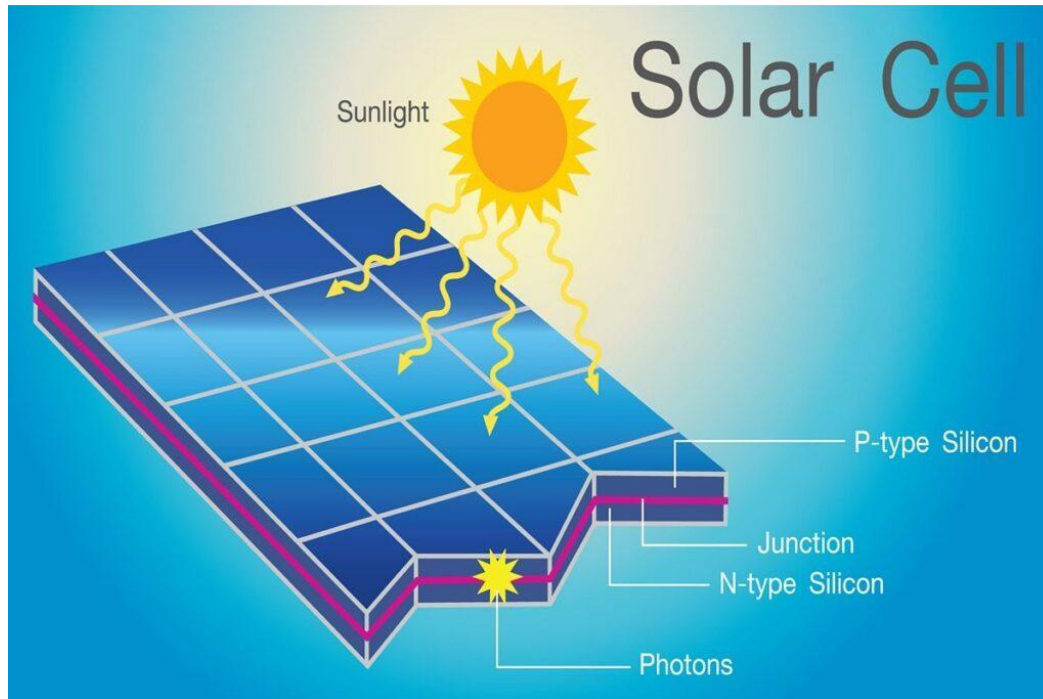


**Figure I.3** Standard solar cell structure [7].

### I.3.1 Window Layer

The window layer is mainly employed to reduce surface recombination. Several conditions must be satisfied when selecting a suitable material for this layer. First, it should possess high transmittance so that most of the incident light can pass through without significant absorption. For this reason, semiconductor materials with a wide band gap are generally preferred.

In addition, the layer must be extremely thin in order to minimize light absorption. To ensure proper contact with the metal electrode, the doping concentration of the window layer should also be higher than that of the p-type region. Figure I.4 presents the energy band diagram between the window layer and the p-region, highlighting its positive effect [8].

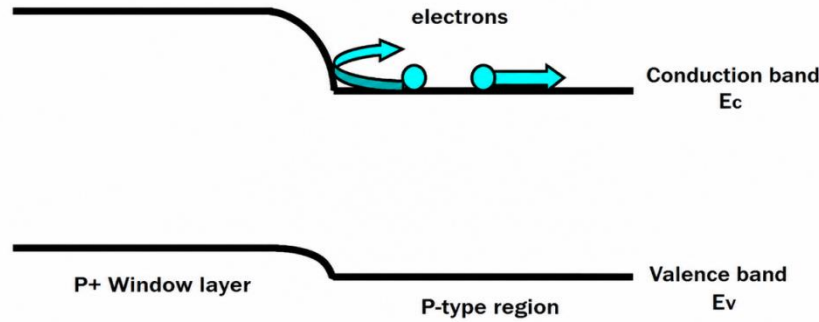


**Figure I.4** Window layer effect [8].

In Figure I.4, the window layer is composed of materials with a wider forbidden band gap than that of the p-type region. Due to its higher doping concentration, this layer can be considered as a  $P^+$  region. At the interface between the window layer and the p-type region, a potential barrier is established for electrons.

This electric field at the  $p^+$  junction helps repel electrons, which are minority carriers in the p region, back toward the depletion zone. Once they reach this region, the internal electric field of the space charge region drives them toward the n-type region.

Thus, the window layer plays an important role in redirecting electrons and reducing the probability of recombination at the upper surface.

### I.3.2 PN Junction

A semiconductor is defined as a material characterized by a band gap ( $E_g$ ) separating the valence band from the conduction band, with the Fermi level located within this forbidden energy gap. The position of the Fermi level depends on the concentration of charge carriers. A semiconductor is considered N-type when electrons are the majority carriers, in which case the Fermi level lies closer to the conduction band. Conversely, it is P-type when holes are the dominant carriers, placing the Fermi level nearer to the valence band [9].

When an N-type semiconductor is brought into contact with a P-type semiconductor, electrons and holes diffuse toward the P and N regions, respectively, in order to achieve charge equilibrium. Holes moving from the P region toward the N region leave behind immobile negative ions, while electrons migrating from the N region toward the P region leave behind

positive charges. As a result, the N region becomes positively charged and the P region becomes negatively charged.

A depletion region, also called the space charge zone (ZCE), is thus formed on both sides of the junction interface, as illustrated in Figure I.5. This region is characterized by an internal electric field directed from the N side toward the P side, creating a potential barrier that opposes further movement of electrons and holes across the junction [6,10].

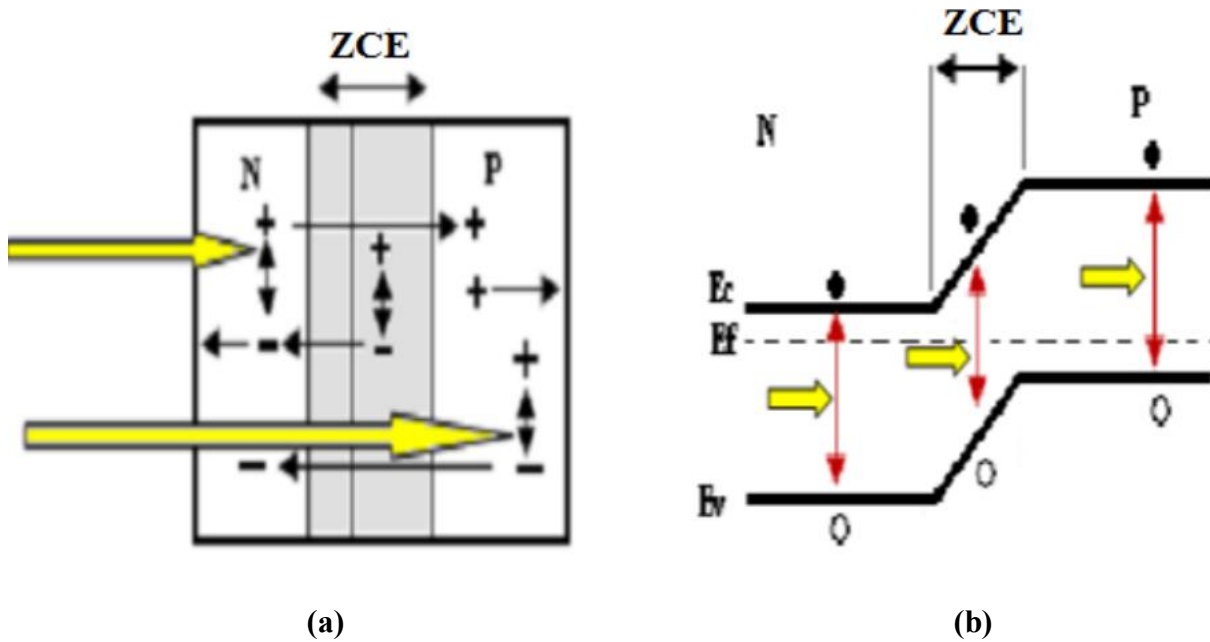


**Figure I.5** a-Structure of a PN junction, b-Band diagram of a PN junction

Junctions formed by the contact of two differently doped regions within the same semiconductor material are called “homo-junctions.” In contrast, junctions created by joining two different semiconductor materials are referred to as “hetero-junctions” [11].

### I.3.3 Back Surface Field (BSF)

At the rear side of solar cells, a metallic contact is required to connect the base region; however, this contact can increase surface recombination rates, which reduces device efficiency. To minimize this effect, recombination can be reduced either by lowering interface defects or by repelling one type of carrier away from the surface. The use of a rear electric field, achieved through a doping gradient [12], has proven to be an effective solution.

The Back Surface Field (BSF) is a heavily doped layer placed at the rear side of the cell and having the same conductivity type as the base (for example, a P<sup>+</sup>/P structure). This

configuration creates a potential barrier that confines minority carriers within the base region, thereby reducing recombination losses, as illustrated in Figure I.5.

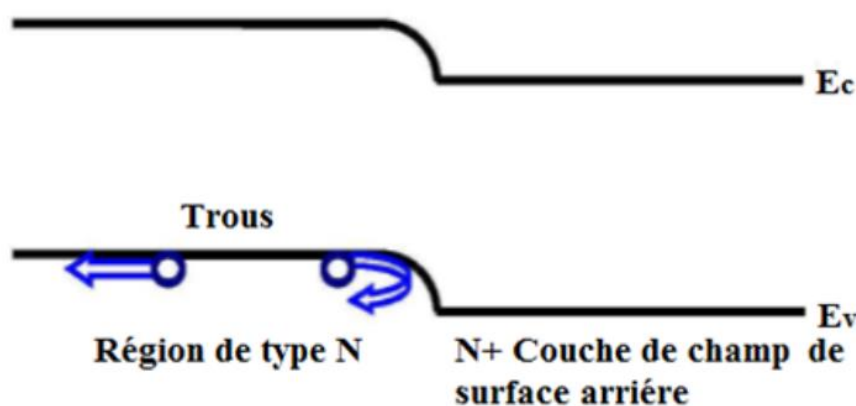


**Figure I.6** Effect of the rear surface field layer [13]

The OSB remains an active field of research, particularly due to the continuous reduction in wafer thickness. In order to save raw material, multicrystalline silicon is now used, offering long minority carrier diffusion lengths [13].

### I.3.4 Front and Rear Face Contacts

Metal contacts (electrodes) are deposited on both sides of the PN junction in order to collect photo-generated carriers and transfer them to the external circuit. For efficient operation, these contacts must be ohmic, ensuring a linear I–V relationship [14].

The resistance associated with these contacts plays a key role in device performance. High contact resistance increases the overall series resistance of the solar cell, which negatively affects the fill factor, the extracted current, and consequently the overall efficiency [15].

On the front side, which is exposed to light, the electrode is designed in a grid pattern to ensure efficient collection of charge carriers while still allowing maximum light transmission. If the grid spacing is too large, more light can enter the cell, but some carriers may recombine before being collected. On the other hand, if the grid is too dense, carrier collection improves, but the amount of incoming light is reduced, which decreases charge generation [16].

In some technologies, transparent and conductive electrodes are used, such as indium tin oxide (ITO) or ZnO. Their optical transparency depends on their band gap, while their

electrical properties are mainly determined by their composition and doping level. Typically, an undoped ZnO layer is first deposited, followed by a doped layer (ZnO:Al or ITO). This intrinsic ZnO layer, which is non-conductive, helps prevent current leakage between the absorber layer and the top contact. In this configuration, a grid structure is no longer required, since this layer covers the entire surface of the cell [16].

On the rear side, a metallic layer is deposited at the bottom of the absorber in order to collect the photo-generated carriers and transfer them to the external load. This layer also serves as a reflector, sending back photons that were not absorbed during their first pass. In conventional solar cells, the back contact material must exhibit low resistivity and enable an efficient flow of majority carriers. This rear contact is becoming more significant as cell thickness decreases, since the carrier generation profile becomes closer to this region.

The main requirements for a back contact material, in addition to good conductivity, are as follows:

- It should form an ohmic contact with the absorber.
- It should present a low recombination rate for minority carriers.
- It should remain chemically stable during subsequent processing steps.
- It should preferably have moderately high reflectivity.

Recombination at the rear contact can become a major limiting factor in device performance. It becomes dominant when the diffusion length becomes comparable to or larger than the absorber thickness [17].

#### **I.4 Operating Principle of a Solar Cell**

A solar cell is made up of several layers, mainly two essential ones: one N-type semiconductor layer and one P-type semiconductor layer. Electrical energy is generated at the junction, also called the metallurgical interface, between these two layers, making it a key component in the field of optoelectronics [18]. These semiconductors are special electronic materials that are sensitive to light and convert solar energy into electrical power through three main processes that occur almost simultaneously.

- a. The absorption of photons (with energy greater than the band gap) by the material of the device.
- b. The conversion of photon energy into electrical energy, which involves the generation of electron-hole pairs in the semiconductor.
- c. The collection of the generated charge carriers within the device [19].

#### a. Light Absorption

Absorption is the first essential step in the photovoltaic conversion process. Light is composed of photons, each carrying a specific amount of energy related to its wavelength. These photons can either penetrate or pass through certain materials depending on their properties.

In general, when a light beam strikes a semiconductor, three main optical phenomena may occur, as illustrated in Figure 1.7:

- **Reflection:** part of the light is reflected from the surface of the material.
- **Transmission:** light passes through the material without being absorbed.
- **Absorption:** light enters the material and is not re-emitted; its energy is converted into another form, usually thermal energy [20].

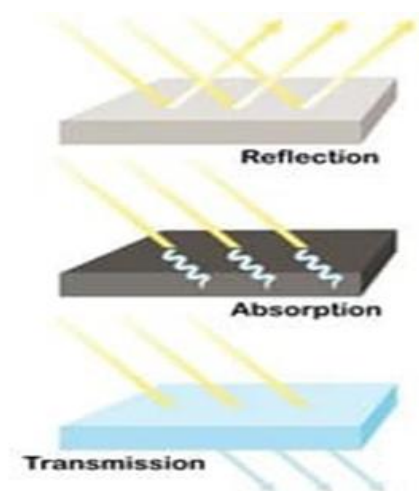


**Figure I.7** Absorption, reflection and transmission phenomena [20].

Indeed, to have a higher yield, the material should have a coefficient

Higher absorption and a low reflection coefficient. In addition, for any beam

luminous which passes through a solid material of thickness ( $l$ ), gives rise to a transmitted beam ( $I$ ) According to the Beer-Lambert law given by the expression (I.4):

$$I = I_0 e^{-\alpha l} \quad [I.4]$$

$I_0$ : Incident beam

$\alpha$ : absorption coefficient

$l$ : The material thickness.

The transmittance and absorbance  $T$  and  $A$  are expressed as follows:

$$T = \frac{I}{I_0} = e^{-\alpha l} \quad [I.5]$$

$$A = -\log_{10}\left(\frac{I}{I_0}\right) = -\log_{10}(T) \quad [I.6]$$

The optical density is given by:

$$DO = -\log_{10}\left(\frac{I}{I_0}\right) = 0.43\alpha l \quad [I.7]$$

The optical density, expressed in equation (I.7), is a parameter that describes the reduction in light intensity as it passes through an absorbing material. It depends on the absorption coefficient  $\alpha$  as well as the thickness of the material [21].

### **b. Conversion of photon energy into electrical energy**

A solid material is composed of atoms made up of a nucleus surrounded by electrons in orbit. The charge carriers responsible for electrical current under illumination are the electrons present in the semiconductor. When a photon is absorbed by the material, it transfers its energy through collision with a peripheral electron, which becomes excited and is released from its initial stable state.

This electron, originally at a lower energy level, moves to a higher energy state, creating a disturbance in the material that results in the formation of an electron-hole pair, both carrying electrical energy [22]. The generation of these free carriers corresponds to transitions between the valence band and conduction band (Bv–Bc) or between specific energy levels and the bands [23]:

- Transition of an electron from the valence band to the conduction band, resulting in the creation of an electron-hole pair.

- Transition from a donor energy (ED) level located within the band gap to the conduction band, leaving behind a positively charged ion and an electron in the conduction band.
- Transition from the valence band to an acceptor energy (EA) level in the band gap, leaving a negatively charged fixed charge and a hole in the valence band.

The electron-hole pair can generate an electric current if it is collected before recombination. Otherwise, it rapidly returns to equilibrium by converting its electrical energy into thermal energy [4].

A photon with frequency  $\nu$  carries an energy  $h\nu$ . When this energy is at least equal to the band gap  $E_g$ , it can be used to excite an electron from the valence band to the conduction band, as shown in equation (I.8).

$$h\nu = h \frac{c}{\lambda} \geq E_g \quad [\text{I.8}]$$

$\lambda$ : the photon wavelength

$c$ : the speed of light

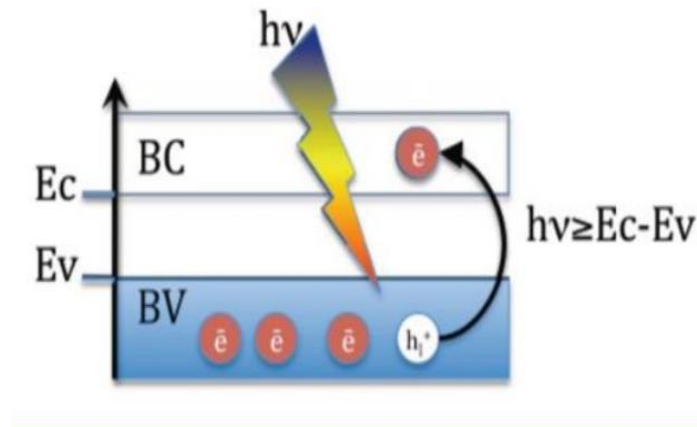


**Figure I.8** Mechanism of creation of an electron-hole pair by a photon [22]

### c. Mechanism of Electron–Hole Pair Generation and Charge Collection

A solar cell is based on a PN junction and operates under illumination. When photons reach the cell, they generate charge carriers in the P-type region, the N-type region, and also within the space charge region (ZCE). These carriers then move toward the depletion region under the influence of the internal electric field. In this region, electron–hole pairs are separated, which improves the charge collection efficiency.

The total photocurrent ( $I_{ph}$ ) is obtained from the combination of the diffusion current, produced by mobile carriers, and the generation current, resulting from the separation of electron–hole pairs in the space charge region. This photocurrent is directly proportional to the incident light intensity.

When the solar cell is connected to an external load, the photogenerated electrons flow through the external circuit and recombine with holes, producing an electric current. The diffusion length ( $L_d$ ) describes the average distance a charge carrier can travel before recombination and is an important parameter in the electron–hole transport process [22].

$$L_d = \sqrt{D\tau} \quad [I.9]$$

It is related to the diffusion coefficient  $D$  and the average lifetime  $\tau$  of minority carriers. It represents the distance over which minority carriers can reach the space charge region (ZCE) before recombining; carriers generated beyond this distance are lost due to recombination [24].

#### **I.4.1 Current–Voltage (I–V) Characteristics of a Solar Cell**

The performance of a solar cell is evaluated using its current–voltage (I–V) characteristic, which provides important information about key parameters such as efficiency, parasitic resistances, and the fill factor. This curve also allows the adjustment and optimization of physical parameters of the cell, including doping levels and layer thicknesses.

The current is measured as a function of the applied voltage, both in the dark and under illumination. Under illumination, the I–V curve shifts downward into the fourth quadrant due to the photocurrent generated by the device, which enables power generation [25].

#### **I.4.2 Ideal Current–Voltage (I–V) Characteristic**

The I-V characteristic of an ideal photovoltaic cell, illustrated in Figures I.9 and I.10, is described by equation (I.10). This model is known as the single-diode exponential model, where the solar cell is represented using one ideal diode.

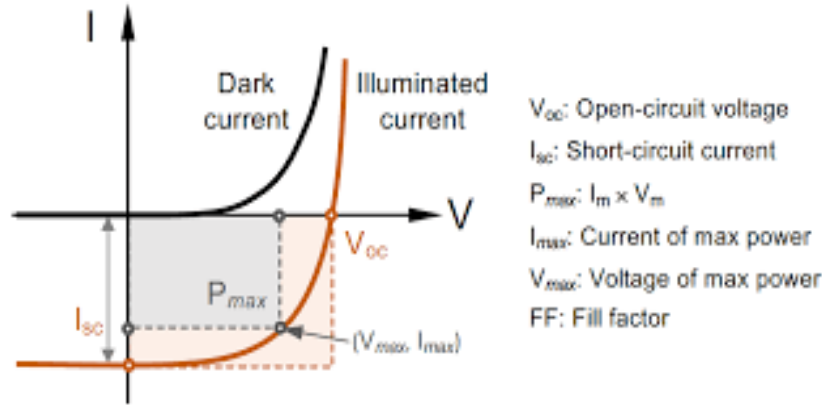


**Figure I.9** Characteristic (I-V) of a solar cell in darkness and under illumination [25].

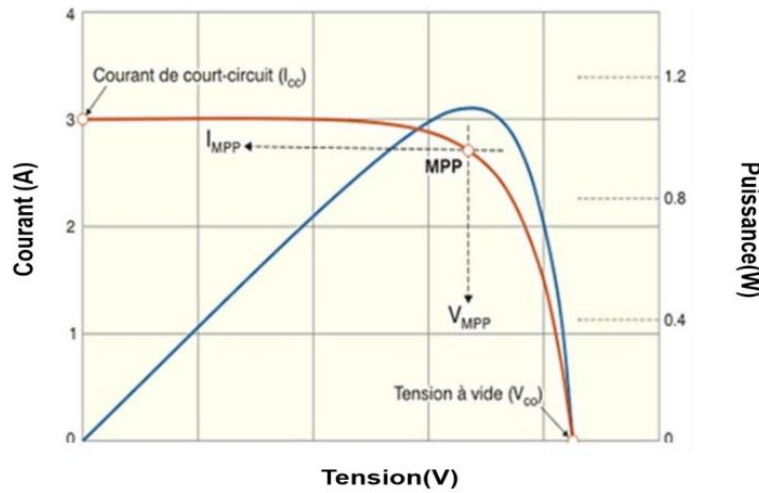


**Figure I.10** Characteristic (I-V) and (P-V) of a solar cell [25].

Under dark conditions, the I-V characteristic of the solar cell behaves like that of a standard diode. When the cell is illuminated, the photocurrent ( $I_{ph}$ ) generated by light is added to the dark current ( $I_{obsc}$ ) of the cell, modifying its overall electrical behavior.

$$I(V) = I_{ph} - I_{obsc} = I_{ph} - I_s \left( \exp\left(\frac{eV}{KT}\right) - 1 \right) \quad (I.10)$$

$$\text{OU} \quad I_s = \left( \frac{D_p n_i^2}{L_p N_D} + \frac{D_n n_i^2}{L_n N_A} \right) \quad (I.11)$$

- $I_{ph}$  Photo-generated current [A]

- $I_{\text{obs}}$  current from the diode to dark [A]
- $V$  Voltage at the terminal of the diode in [V]
- $e$  Elementary charge of an electron ( $e = 1.602 \times 10^{-19}$  C)
- $K$  Boltzmann constant ( $k = 8.62 \times 10^{-5}$  eV. K<sup>-1</sup>)
- $T$  Temperature in Kelvin
- $n_i$  Intrinsic constant
- $I_s$  Diode saturation current in (A)

$D_n$  and  $D_p$  represent the diffusion coefficients of minority carriers in the N-type and P-type materials, respectively.

- $L_n$  and  $L_p$  correspond to the diffusion lengths of minority carriers in the N and P regions, respectively.

The equivalent electrical circuit of an ideal solar cell based on a PN junction can be modeled by a diode, which represents the junction behavior, in parallel with a current source  $I_{\text{ph}}$ , which represents the photogenerated current, as shown in Figure (I.11) [26].

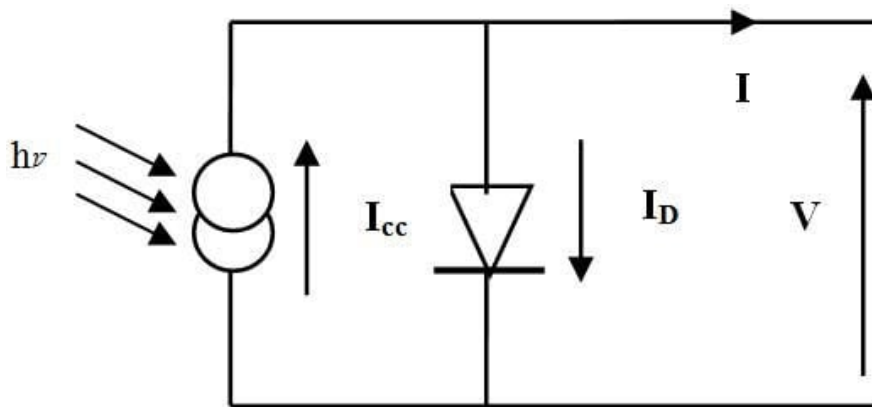


**Figure I.11** Equivalent diagram of an ideal solar cell

### I.4.3 Current–Voltage (I–V) Characteristics in the Real Case

In practice, the single-diode model described by equation (I.10) does not fully represent the actual behavior of a solar cell. This is mainly because it neglects the effects of series and

shunt (parallel) resistances, which originate from the electrical contacts on the carrier-collecting materials that are not perfectly ohmic.

In addition, this simplified model does not account for electron–hole recombination within the space charge region (ZCE), which is caused by localized energy states in the band gap and leads to a reduction in the output current. This recombination effect can be represented by introducing a second diode in parallel.

By considering these non-ideal effects, the current of a real solar cell can be described using the two-diode model given in equation (I.12), which provides a more accurate representation of the actual device behavior.

$$I(V) = I_{ph} - I_{s1} \left( \exp\left(\frac{e(V+IR_s)}{n_1 KT}\right) - 1 \right) - I_{s2} \left( \exp\left(\frac{e(V+IR_s)}{n_2 KT}\right) - 1 \right) - \frac{V+IR_s}{R_p} \quad (I.12)$$

- $I_{s1}$  and  $I_{s2}$  Saturation current of the diode D1 and D2 [A].
- $n_1$  and  $n_2$  Ideality factor for diodes D1 and D2.
- $R_s$  serial resistance [ $\Omega$ ].
- $R_p$  parallel resistance [ $\Omega$ ].

The equivalent electrical circuit of the cell, shown in Figure I.12, includes a current source that represents the photogenerated current. The overall resistive losses of the device are modeled by a series resistance ( $R_s$ ) and a shunt (parallel) resistance ( $R_p$ ).

Diode ( $D_1$ ) represents the current contribution from the n-type emitter and the p-type base of the solar cell, while the second diode ( $D_2$ ), also connected in parallel, accounts for the generation–recombination processes occurring within the space charge region [26].

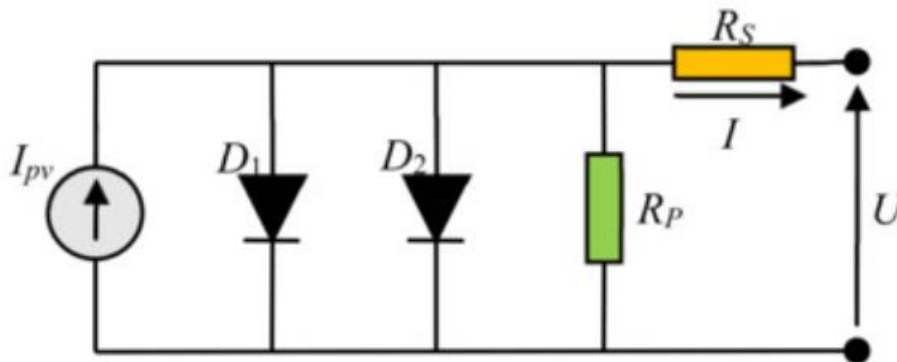


**Figure I.12** Equivalent electrical diagram of a photovoltaic solar cell taking in counts the different losses based on the two-diode model

It is possible to simplify this model by removing the second diode associated with recombination in the space charge region (ZCE), and by introducing an ideality factor, as shown schematically in Figure (I.13).

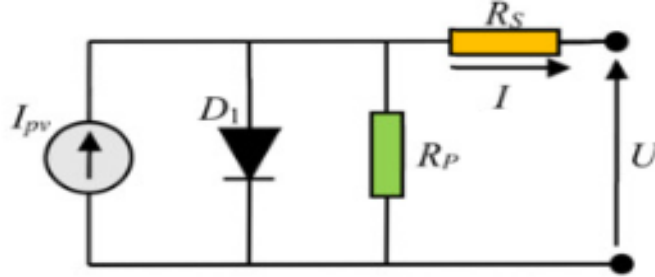


**Figure I.13** Equivalent diagram of a solar cell to a diode with losses and a coefficient of ideality

The current  $I$  can then be expressed as a function of the voltage  $V$ , generally using the following expression (I.13):

$$I(V) = I_{ph} - I_s \left( \exp\left(\frac{e(V+IR_s)}{n_{id} KT}\right) - 1 \right) - \frac{V+IR_s}{R_p} \quad (I.13)$$

With

- $I_s$  : Saturation current (A).
- $R_s$ : Series resistance ( $\Omega$ ).
- $R_p$ : Parallel resistance ( $\Omega$ ).
- $n_{est}$ : Diode ideality coefficient,  $n_{est} \approx 1$ .
- $I_{ph}$ : Photo-generated current.

The series resistance  $R_s$  represents the resistive losses within the structure, including losses at the metal/semiconductor interfaces and in the metallic contacts themselves. The slope of the I–V curve at the open-circuit voltage point  $V_{oc}$  is equal to the inverse of  $(1/R_s)$ . To reduce its effect on the cell current, it is important to minimize  $R_s$  by improving the metal/semiconductor contacts and decreasing the material resistivity. However, an appropriate compromise must be maintained, since excessive doping may increase recombination effects. In practice, substrate resistivities are usually between 0.5 and 5  $\Omega \cdot \text{cm}$  [27,28].

The parallel resistance  $R_p$  models surface leakage currents and losses caused by material defects. Consequently, part of the photocurrent  $I_{ph}$  flows through this resistance instead of reaching the external load. The slope of the  $I(V)$  curve at the short-circuit current point  $I_{cc}$  corresponds to the inverse of the parallel resistance ( $(1/R_p)$ ) [29].

Figure (I.14) shows the variation of the  $I(V)$  characteristic according to the values of  $R_s$  and  $R_p$ . a steeper slope of the current–voltage curve at  $(V = V_{oc})$  indicates a low series resistance, which improves the fill factor and overall device performance. In contrast, a more pronounced slope at  $(I = I_{cc})$  indicates a low parallel resistance, leading to a reduction in the fill factor and consequently a decrease in performance [29].

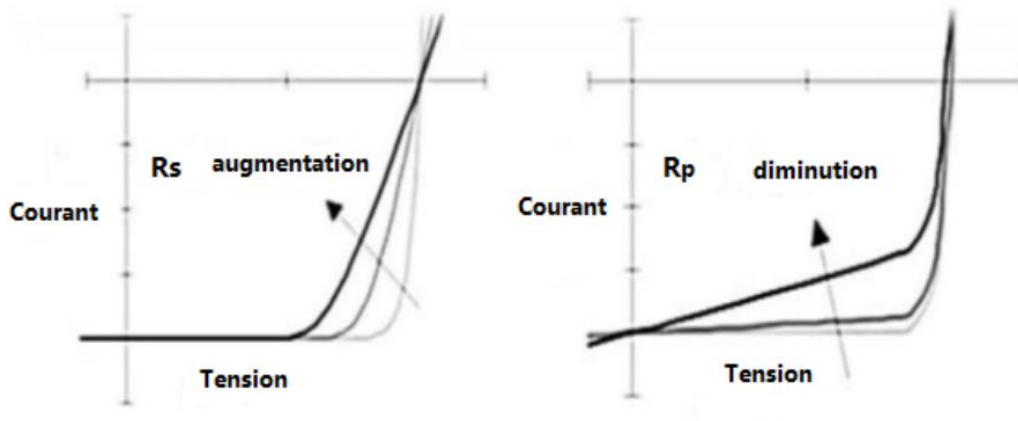


**Figure I.14** Theoretical effect of the series resistance and the parallel resistance of a cell solar PV on its curve ( $I$ - $V$ )

## I.5 Photovoltaic Parameters of a Solar Cell

The illuminated  $I$ - $V$  curve, presented in Figure I.10, shows the different possible operating conditions of a solar cell. From this characteristic, the operation of the cell can be analyzed using four main photovoltaic parameters: the short-circuit current, the open-circuit voltage, the fill factor, and the maximum power. In addition, the spectral response and electrical efficiency can also be examined to evaluate the overall performance of the cell [30].

### I.5.1 Short-Circuit Current ( $I_{cc}$ )

The short-circuit current, denoted ( $I_{cc}$ ), and expressed in mA (or in mA/cm<sup>2</sup> as current density), is the current delivered by the cell when the applied voltage is zero ( $(V = 0)$ ). It mainly depends on the light intensity, through the photogenerated current ( $I_{ph}$ ), as well as on the surface area of the cell [6].

This current increases linearly with the illumination intensity and is influenced by several factors such as the illuminated surface, the wavelength of the incident radiation, the mobility of charge carriers, and the temperature.

For an ideal solar cell, the short-circuit current ( $I_{cc}$ ) is equal to the photocurrent  $I_{ph}$ . It represents the number of generated electron–hole pairs that successfully pass through the junction without recombination [14].

$$I_{cc} = I_{ph} = qG(L_n + L_p) \quad (I.14)$$

Where

- $L_n, L_p$ : The diffusion lengths of electrons and holes respectively.
- $G$ : the generation rate.
- $q$ : Elementary charge [21].

### **I.5.2 Open-Circuit Voltage ( $V_{co}$ )**

When the solar cell operates under open-circuit conditions, the charge carriers generated by light and separated by the internal electric field accumulate on both sides of the junction. This situation corresponds to the maximum voltage across the cell when no current flows ( $I = 0$ ), meaning the voltage produced by an illuminated cell that is not connected to an external circuit.

This voltage depends on the difference in the work functions of the electrodes as well as the shunt resistance. It decreases as temperature increases and also varies with the intensity of the incident light [14]. It can be determined using the following relation:

$$V_{co} = \frac{KT}{vq} \ln\left(\frac{I_{ph}}{I_s} + 1\right) \quad (I.15)$$

Where:

- **K**: Boltzmann constant
- **T**: absolute temperature
- **q**: electric charge
- **$I_s$** : saturation current [4]

### I.5.3 Maximum Power Pmax

The power delivered by a solar cell reaches its maximum at a specific operating point on the I–V characteristic. This point, noted  $P_m(V_m, I_m)$ , is located at the knee of the I–V curve and is called the maximum power point (MPP). The corresponding values  $V_m$  and  $I_m$  are referred to as the maximum voltage and maximum current, respectively [31].

$$P_{\max} = I_{\max} \cdot V_{\max} \quad (I.16)$$

In the case of an ideal solar cell, the maximum power corresponds to the product of the open-circuit voltage  $V_{co}$  and the short-circuit current  $I_{cc}$ .

$$P_{\max \text{ idéal}} = I_{cc} \cdot V_{co} \quad (I.17)$$

### I.5.4 Fill Factor (FF)

An important parameter commonly extracted from the I–V characteristic is the fill factor (FF), which is used to evaluate the quality of a photovoltaic cell. It is defined as the ratio between the maximum power delivered ( $P_{\max}$ ) and the product of the short-circuit current ( $I_{cc}$ ) and the open-circuit voltage ( $V_{co}$ ). The fill factor is always less than 1 and is given by the following expression [32]:

$$FF = \frac{P_{\max}}{I_{cc} V_{co}} = \frac{I_m V_m}{I_{cc} V_{co}} \quad (I.18)$$

Mathematically, the fill factor can also be expressed in terms of the open-circuit voltage or as a function of the series and shunt resistances of the solar cell. For an ideal solar cell, this parameter depends mainly on the open-circuit voltage. It is given by equation (I.19), which depends only on the normalized voltage  $V_{co} = V_{co} / K_B T$  [33].

$$FF_0 = \frac{V_{co} - \ln(V_{co} + 0.72)}{V_{co} + 1} \quad (I.19)$$

In practical conditions, the fill factor is highly influenced by the parasitic resistances  $R_s$  and  $R_{sh}$  of the solar cell [34].

$$FF = FF_0 (1 - r_s) \quad (I.20)$$

$$r_s = \frac{R_s I_{cc}}{V_{co}} \quad (I.21)$$

### I.5.5 Electrical Efficiency $\eta$ :

The conversion efficiency is a key parameter used to evaluate the performance of a solar cell. It represents the ability of the device to effectively convert incident light photons into electrical energy. It is defined as the ratio between the output power  $P_{out}$  and the input power  $P_{in}$ , which corresponds to the incident solar radiation.

For terrestrial applications, the AM1.5G solar spectrum is typically used, corresponding to an irradiance of approximately  $1000 \text{ W/m}^2$ . The efficiency is given by the following expression:

$$\eta = \frac{P_{out}}{P_{in}} = \frac{V_{oc} I_{sc} FF}{P_{in}} \quad (\text{I.22})$$

The yield of solar panels is influenced by several external factors such as geographical location, cloud coverage, season of the year, and other environmental conditions [31].

### I.5.6 Spectral Response $R_s$

The spectral response  $R_s$  of a photovoltaic cell is defined as the ratio between the short-circuit current generated by the cell and the incident optical power, depending on the wavelength of the incoming radiation. It describes how effectively the solar cell converts light of different wavelengths into electrical current. The spectral response  $R_s$  is given by the following relation [35]:

$$RS(\lambda) = \frac{I_{sc}(\lambda)}{P_{in}(\lambda)} \quad (\text{A/W}) \quad (\text{I.23})$$

### I.5.7 Internal Quantum Yield (IQE)

The internal quantum yield (IQE) of a solar cell is defined as the ratio between the number of generated charge carriers and the number of photons that actually penetrate into the material. It is related to the external quantum efficiency (EQE) through the following equation [31]:

$$EQE(\lambda) = RS(\lambda) \frac{h.c}{\lambda.e} \quad (\text{I.24})$$

Where  $R(\lambda)$  represents the reflection coefficient as a function of wavelength  $\lambda$ .

## I.6 Different Types of Losses in a Solar Cell

In practice, photovoltaic conversion is not loss-free, which limits the overall efficiency of solar cells. Due to these losses, the theoretical maximum efficiency is about 31%, according to the Shockley–Queisser limit [37]. However, third-generation photovoltaic concepts may increase this limit up to around 44% by making better use of both high- and low-energy photons [38].

The losses that affect efficiency are generally classified into two main categories: optical losses and electrical losses.

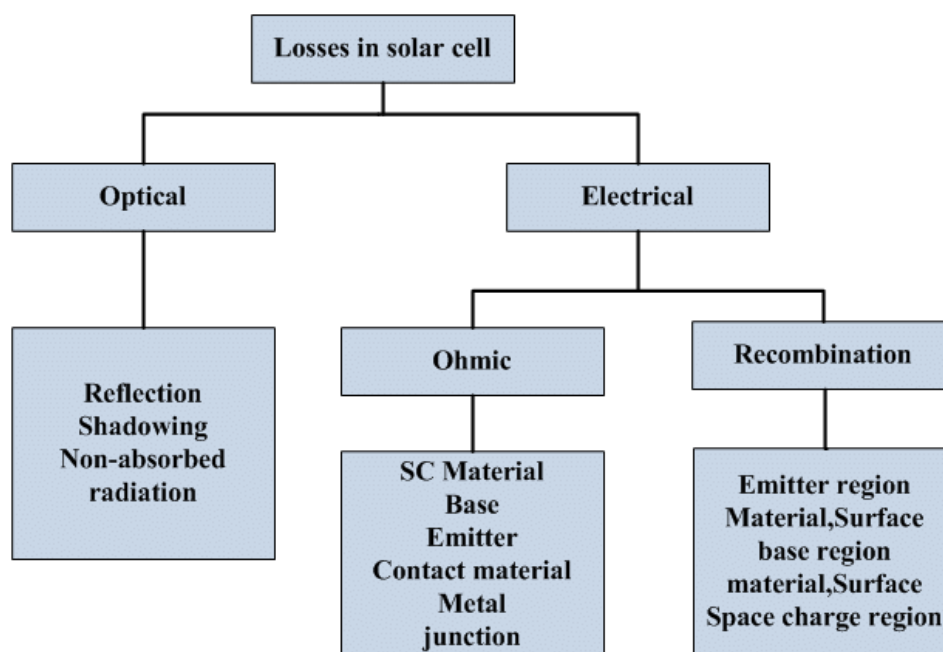


**Figure I.15** Different types of losses in solar cells

### I.6.1 Optical Losses

- Photons with energy lower than the band gap cannot be absorbed by the material and therefore do not contribute to the generation of electron–hole pairs. This results in a loss of approximately 27% of the efficiency (Region A in Figure I.16).
- Photons with energy higher than the band gap also contribute to losses because the excess energy is dissipated through thermalization, meaning it is lost as heat instead of being used for carrier generation. This accounts for about 28% of the total losses (Region B in Figure I.16).

- Reflection losses occur when part of the incident light is reflected by the non-metallized surface of the solar cell, reducing the amount of absorbed radiation.
- Shading losses are caused by the metallic grid on the front surface of the cell, which blocks

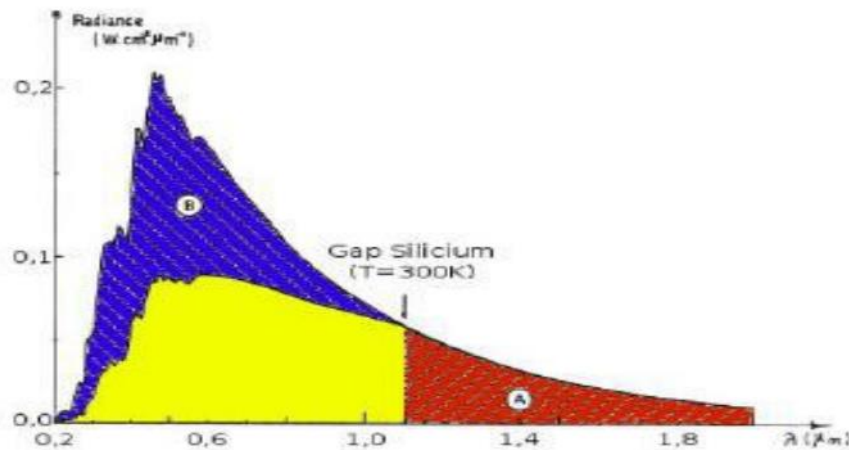


Figure I.16 Optical losses in a silicon-based solar cell [39]

## I.6.2 Electrical Losses

**Resistive losses:** These losses are mainly caused by the series resistance, which reduces the current flowing in the circuit, as well as by shunt (parallel) resistances. These include leakage currents at the edges of the photovoltaic cell or when a metallic contact on the front side creates a short circuit with the emitter.

- **Voltage factor:** The open-circuit voltage cannot exceed the band gap voltage. In practice, it represents only a fraction of this value due to Auger recombination processes, which limit its magnitude [40].
- **Fill factor:** Because of the exponential nature of the current–voltage relationship, an ideal perfectly rectangular  $I(V)$  curve (100%) cannot be achieved. The fill factor (FF) can reach values of up to approximately 89% in optimized cells [40].
- **Recombination losses:** The generated charge carriers must reach the contacts in order to contribute to current generation. However, if they recombine before being collected, they do not contribute to the output current. Several recombination mechanisms exist, both in the bulk and at the surface of the material, affecting electron–hole pairs [41].

### I.6.2.1 Types of Recombination

### I.6.2.1.1 Radiative Recombination

- **Band-to-band recombination:** It occurs when an electron in the conduction band recombines with a hole in the valence band, resulting in the emission of a photon whose energy is close to the band gap of the material.
- **Recombination via impurity levels:**  
In this case, three mechanisms can be distinguished. First, an excited electron from donor levels returns to the valence band. Second, an electron from the conduction band recombines with an acceptor level. Third, an electron from a donor level recombines directly with an acceptor level.
- **Recombination due to isoelectronic traps (excitons):**  
Excitons are neutral states formed when an electron and a hole are bound together. They do not contribute additional charge carriers to the host material [42].

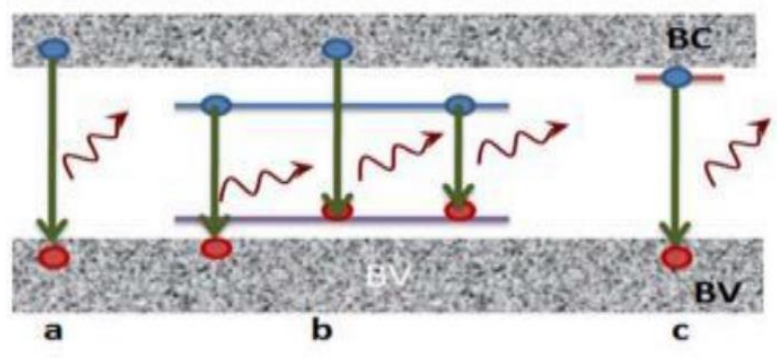


**Figure I.17** Radiative recombination mechanisms: a) band-to-band, b) through impurity levels, c) Due to excitons [42].

### I.6.2.1.2 Non-Radiative Recombination

- **Auger recombination:**  
This process can occur either through a direct band-to-band transition or via a recombination center. In this mechanism, the excess energy is transferred to a third carrier (electron or hole), which is excited to a higher energy state see Figure I.18.a. This energy is then dissipated non-radiatively in the crystal lattice.

- **Shockley–Read–Hall (SRH) recombination:**

This mechanism, which is dominant in most semiconductors, occurs in two steps through a recombination center such as a defect or impurity that introduces a deep energy level  $E_p$  within the band gap see Figure I.18.b [43].

- **The four possible processes involved are:**

1. Capture of an electron by a trap level (transition from  $E_c$  to  $E_p$ ).
2. Emission of an electron from a trap level (transition from  $E_p$  to  $E_c$ ).
3. Emission of a hole from a trap level (transition from  $E_v$  to  $E_p$ ).
4. Capture of a hole by a trap level (transition from  $E_p$  to  $E_v$ ).

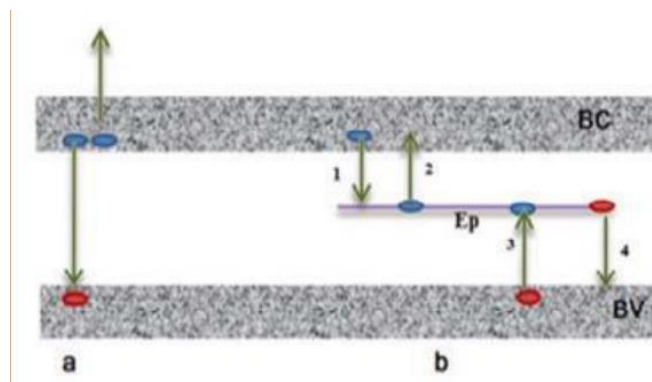


**Figure I.18** Mécanismes de recombinaisons non radiatives : a) de type Auger, b) de type Shockley-Read -Hall (SRH) [43].

## I.7 Photovoltaic Cell Technologies

Over the past decade, photovoltaic energy has become a major player in the transition toward alternative energy sources. This progress has been largely enabled by advances in materials and manufacturing techniques. However, despite these developments, important challenges still remain in achieving cleaner and more cost-effective photovoltaic energy production. Current research is therefore focused on high-efficiency solar cell structures such as multi-junction cells, graphene-based devices, intermediate band cells, as well as materials suitable for printing technologies, including quantum dots [44].

The fabrication of photovoltaic cells relies on various technologies that tailor the properties of materials in order to enhance photoelectric conversion efficiency across the different components of the cell. The development and use of innovative and non-traditional

manufacturing approaches have led to the classification of photovoltaic technologies into four main generations, as shown in Figure I.19 [45].

This classification reflects the historical evolution of solar cells since their invention. In recent decades, four main generations have been identified:

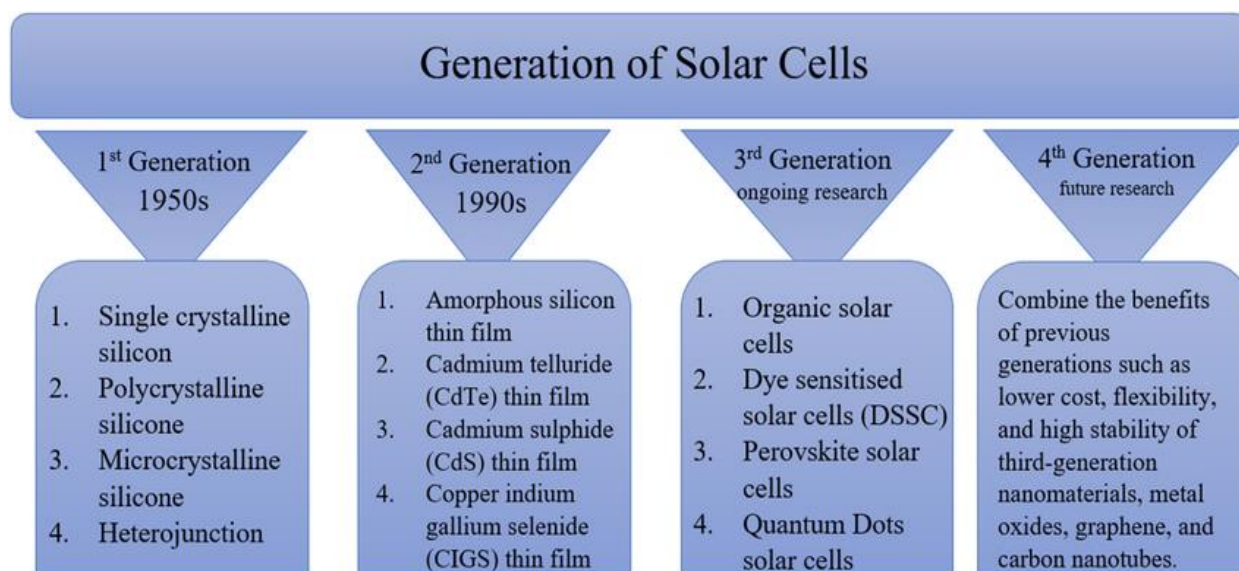


**Figure I.19** Different generations of photovoltaic cells

### ► Third Generation

In order to overcome the limitations of previous generations—such as high manufacturing costs, limited material availability, and material toxicity—several concepts have been proposed, leading to the development of third-generation solar cells. These technologies are still mainly at the research stage, but they show very promising potential for addressing these challenges in the near future. Among them, multi-junction cells are particularly important in this study.

### ► Multi-junction Cells

It is often difficult to find a single material capable of absorbing the entire solar spectrum with a high absorption coefficient. III–V multi-junction cells provide a solution to this problem. They use a stacked structure composed of multiple layers with different band gaps arranged in decreasing order, where each junction is optimized to absorb a specific portion of the solar spectrum efficiently. This approach helps to reduce thermalization losses and allows better

utilization of almost the entire solar spectrum, resulting in very high conversion efficiencies [24,48].

Multi-junction photovoltaic cells based on III–V semiconductor combinations (such as GaAs, AlGaAs, InGaAs, etc.) have been developed since the 1960s and can achieve very high efficiencies, sometimes exceeding 40% under concentrated sunlight [24]. These cells are mainly used in the space industry due to their high cost, making them unsuitable for widespread domestic applications. However, their performance depends strongly on operating conditions, as concentrated sunlight must continuously be focused on the cell. For this reason, solar tracking systems are required to maintain optimal alignment with the sun and ensure efficient current generation [24].

## **I.8 Conclusion**

In this chapter, the fundamental principles required to understand solar cells were established. First, several concepts related to the Sun as an energy source were introduced. The study then focused on the photovoltaic effect, the operating principle of photovoltaic cells, and their I–V characteristics under both dark and illuminated conditions, as well as the key parameters that influence their performance.

The next chapter will focus on the simulation tools used in this work, particularly the **(SCAPS-1D)** . It will present the software environment, its operating principles, and the different device structures adopted for the simulations carried out in this study.

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## II.1 Introduction

In the previous sections, we discussed the theoretical concepts of photovoltaics, including its definition and history. We also presented the solar spectrum and solar radiation used, and described the operating principle of photovoltaic cells

In this part, we study some types of solar cells using the SCAPS simulator. We also present a brief overview of this software. In addition, we introduce some key concepts and provide a detailed explanation of how to define and simulate a solar cell using this tool.

## II. 2 Definition

SCAPS (Solar Cell Capacitance Simulator) is a numerical simulation software used for one-dimensional solar cells, developed by the Department of Electronics and Information Systems (ELIS) at Ghent University in Belgium. The development of this software has involved contributions from several researchers: Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraegen, and Stefaan Degraeve have contributed to the development of this software [1]. The software is freely accessible to the photovoltaic research community, including research centers and academic institutions. It operates on Windows systems such as Windows 95, 98, NT, 2000, XP, Vista, Windows 7, and Windows 8, and requires around 50 MB of disk space. SCAPS was initially developed for CuInSe<sub>2</sub> and CdTe-based cell structures. However, several extensions have expanded its capabilities, allowing it to be used for crystalline solar cells (such as Si and GaAs) as well as amorphous solar cells (a-Si and micro-morph Si). An overview of its main features is presented below : Up to 7 semiconductor layers. Almost all parameters can be defined with graded variations depending on the composition and depth of the cell. For example:

Recombination mechanisms: band-to-band (direct), Auger, SRH. Defect levels: in the bulk or at the interface, taking into account their charge states and recombination processes at these levels.

- Defect levels and charge types: neutral (uncharged), monovalent (single donor or acceptor), divalent (double donor or acceptor, amphoteric), and multivalent (user-defined).
- Defect levels and energy distribution: discrete levels, uniform distribution, Gaussian distribution, tail-like distribution, or a combination of these distributions.

- Defect levels and optical properties: direct light excitation is possible, known as the impurity photovoltaic (IPV) effect

- . • Defect levels and metastable transitions between different energy levels.
- Contacts: metal work function or flat-band condition; optical properties of the filter, including reflection and transmission.
- . Tunneling: includes inter-band tunneling in both the conduction and valence bands, as well as tunneling through interface states.
- . Generation: can be performed either through internal calculations or by importing a user-defined  $g(x)$  file.
- . Illumination: multiple spectral options are supported, such as AM0, AM1.5D, AM1.5G, AM1.5G Edition 2, monochromatic, white light, and others.
- . Illumination may be applied from either the p-side or the n-side of the device.
- . Additional functionalities are discussed in more detail in the software manual [1].

### II.3. Basic Concepts

SCAPS is a software program developed for the Windows operating system using LabWindows/CVI from National Instruments. The program launches through the “Action Panel” icon, after which the following window appears:

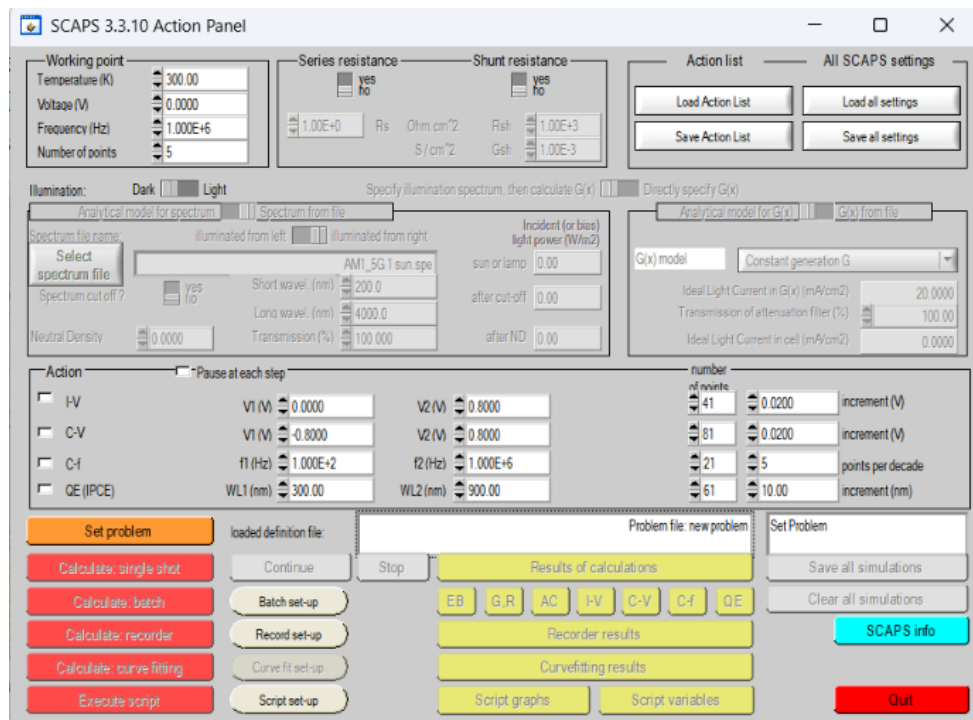


**Figure II.1** The SCAPS Start-Up Panel and the Main Action Panel.

### II. 3.1 Launching SCAPS

To start SCAPS, click the desktop icon or double-click the *SCAPS3310EXE* file in the file manager (or any other SCAPS version). The software will then open with the Action Panel.

### II. 3.2 Defining the Operating Point

The operating point determines the parameters that stay fixed during the simulation measurements and are associated with the operating conditions. This includes:

- **Temperature T:** an essential parameter for all measurements.  
**Note:** In SCAPS, only the thermal velocities and the temperature of the photovoltaic cell (or device) can be manually modified by increasing or decreasing them to the required value.
- **Voltage V:** It is not relevant to I–V and C–V simulations. It corresponds to the DC bias voltage in a C–f simulation. SCAPS simulations begin at 0 V and then advance to the operating-point voltage through a defined number of steps.
- **Frequency F:** It is not associated with I–V and C–f simulations. It corresponds to the frequency used for simulating the C–V characteristic.

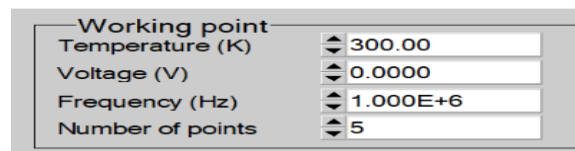


Figure II.2 working point

**Number of points:** corresponds to the number of points used for plotting the curves.

### II. 3.3 Series Resistance and Shunt (Parallel) Resistance

To enable the series and shunt resistances, simply select the “Yes” box. Both parameters can be adjusted manually by increasing or decreasing their values. These two parameters affect the I–V characteristic.

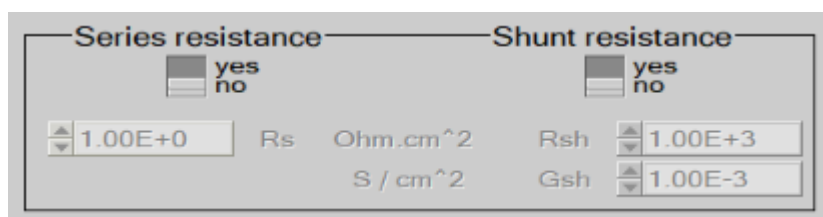


Figure II.3 series and shunt resistance block

### II. 3.4 Light Source

Simply click the “Light” button to turn on the light source.

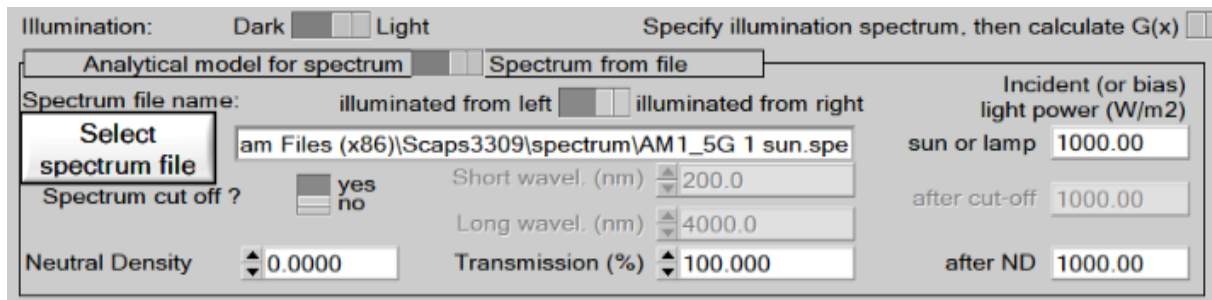


**Figure II.4** Light Illumination Block.

This block is used to manage the illumination parameters through specific fields, namely the activation of the light source, the monochromatic or polychromatic spectrum, and the wavelength range, including solar illumination, etc.

### II.3.5 Illumination

Illumination is applied in all measurements. It defines the light polarization conditions. The basic parameters include dark or light conditions, the choice of the illuminated side, and the selection of the spectrum. The illumination spectrum, one Sun (1000 W/m<sup>2</sup>) with global air mass 1.5, is used as the default spectrum. However, a wide variety of monochromatic light sources and spectra are also available for more specific simulations. When an optical simulator is available, a generation profile can be imported directly instead of selecting a spectrum.

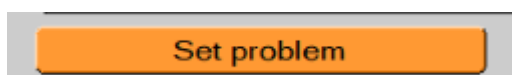
### II. 3.6 Action

This block allows us to define the magnitudes needed for simulation. To do so, each magnitude must be verified against the specific quantity to be simulated, enabling the determination of characteristics such as current–voltage (IV), capacitance–voltage, capacitance–frequency, and spectral response.

| Action                             |                                               | <input type="checkbox"/> Pause at each step   |                                         | number of points                |                                                   |
|------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------|---------------------------------|---------------------------------------------------|
| <input type="checkbox"/> I-V       | V1 (V) <input type="text" value="0.0000"/>    | V2 (V) <input type="text" value="0.8000"/>    | <input type="checkbox"/> Stop after Voc | <input type="text" value="41"/> | <input type="text" value="0.0200"/> increment (V) |
| <input type="checkbox"/> C-V       | V1 (V) <input type="text" value="-0.8000"/>   | V2 (V) <input type="text" value="0.8000"/>    |                                         | <input type="text" value="81"/> | <input type="text" value="0.0200"/> increment (V) |
| <input type="checkbox"/> C-f       | f1 (Hz) <input type="text" value="1.000E+2"/> | f2 (Hz) <input type="text" value="1.000E+6"/> |                                         | <input type="text" value="21"/> | <input type="text" value="5"/> points per decade  |
| <input type="checkbox"/> QE (IPCE) | WL1 (nm) <input type="text" value="300.00"/>  | WL2 (nm) <input type="text" value="900.00"/>  |                                         | <input type="text" value="61"/> | <input type="text" value="10.00"/> increment (nm) |

Figure II.5 action block

### II.3.7 Define the Problem



In the Action panel, click the **SET PROBLEM** button and then select **LOAD** from the lower right corner of the panel that appears. Open a file, for example, **NUMOS CIGS Baseline.def**, which serves as a sample for a CIGS-based solar cell.

After loading, all the cell properties can be modified by clicking **SET PROBLEM** again in the Action panel.



Figure II.6 set problem

### II.3.8 Selection of the Characteristics to Be Simulated

Within the Action section of the Action panel, you can choose one or more characteristics to simulate, such as IV, CV, or Cf. You can also specify the variable's starting and ending values, along with the number of steps for the simulation.

### II. 3.9 Solar cell definition panel

Clicking the “**SET PROBLEM**” button in the Action panel opens the window shown in Figure IV-13, known as the Solar Cell Definition Panel.

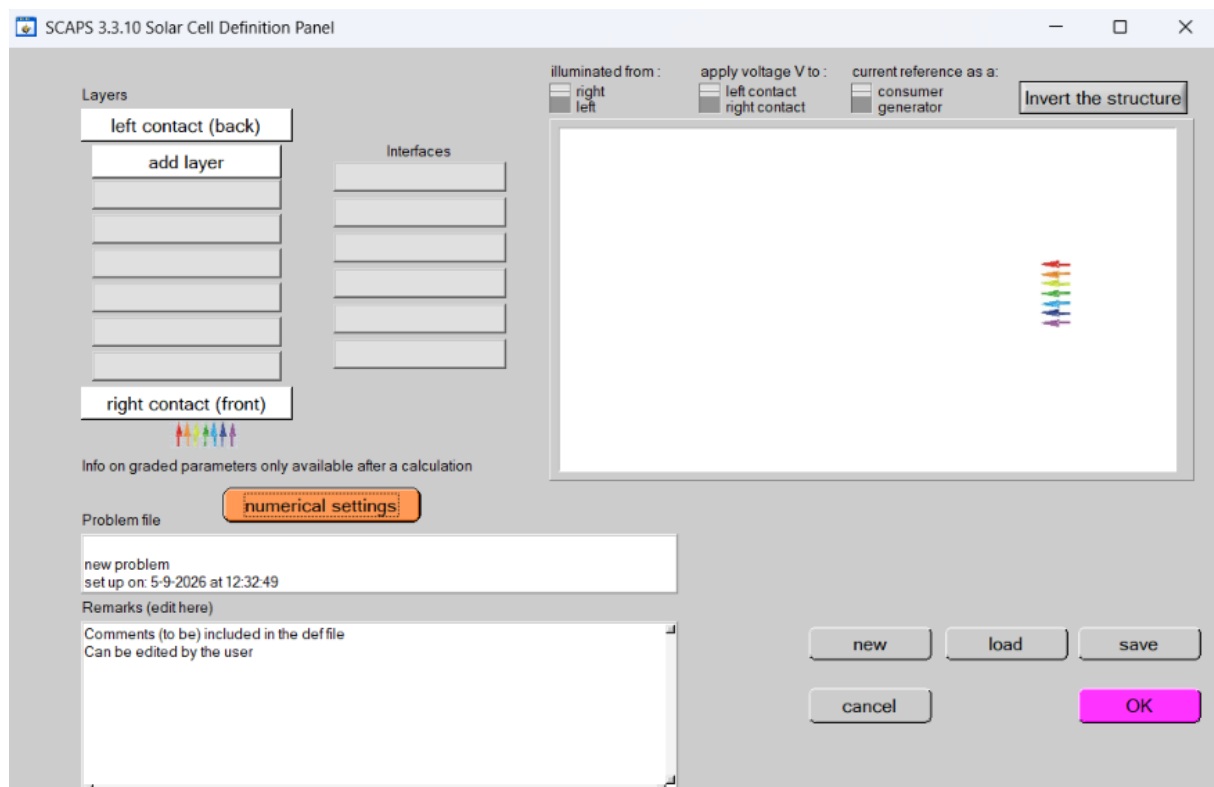


Figure II.7 solar cell identification plate

- a- **New:** allows the creation of a new photovoltaic device.
- b- **Add a Layer:** opens a window with fields to complete using the parameters that characterize the layer under study, namely: the layer name, thickness, band gap energy, electron affinity, electrical permittivity, mobility, and doping type. Finally, click on “**Add.**”

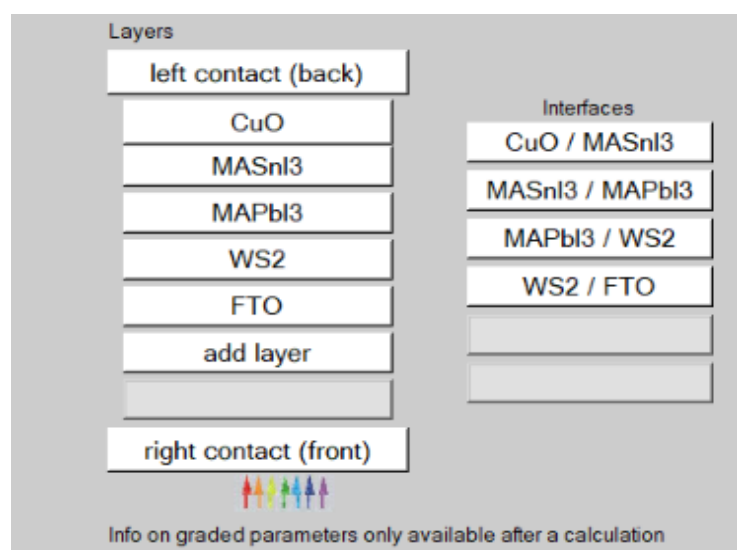


Figure II.8 Definition of the structure of a solar cell

### II.3.10 – Contacts

The contact properties can be defined by clicking either the front contact button or the rear contact button in the Cell Definition Panel. A panel named “**CONTACT PROPERTIES PANEL**” then appears, as shown in Figure II.9.

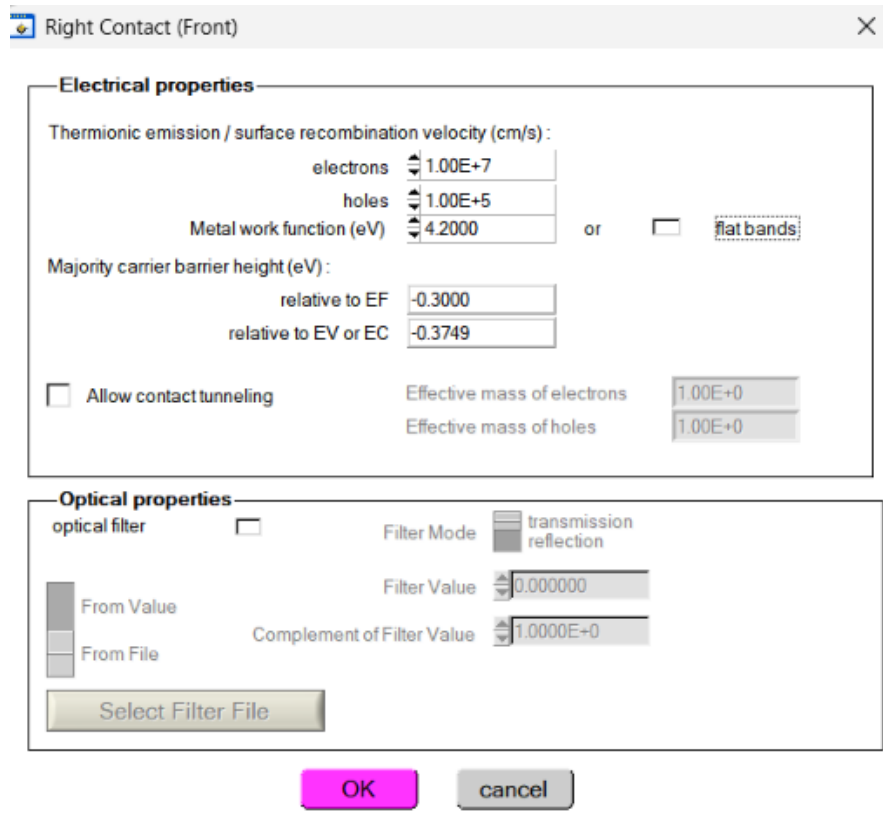


**Figure II.9** right contact (front)

The contact properties are classified into electrical and optical properties. For the electrical properties, the following parameters can be defined:

- . The surface recombination rates of electrons and free holes. If the contact has a work function, it is treated as ideal (flat-band regime).
- . The majority carrier barrier.
- . The tunneling effect (if considered in the simulation).

Regarding the optical properties, the transmission or reflection can be specified either by a fixed value or through a data file.

### II.3.11 – Definition of Layers

By clicking the “**Add Layer**” button, a window (Fig.II.10) appears containing the various

parameters of the material to be introduced. These parameters can be defined with either uniform or non-uniform distributions, depending on the material physics.

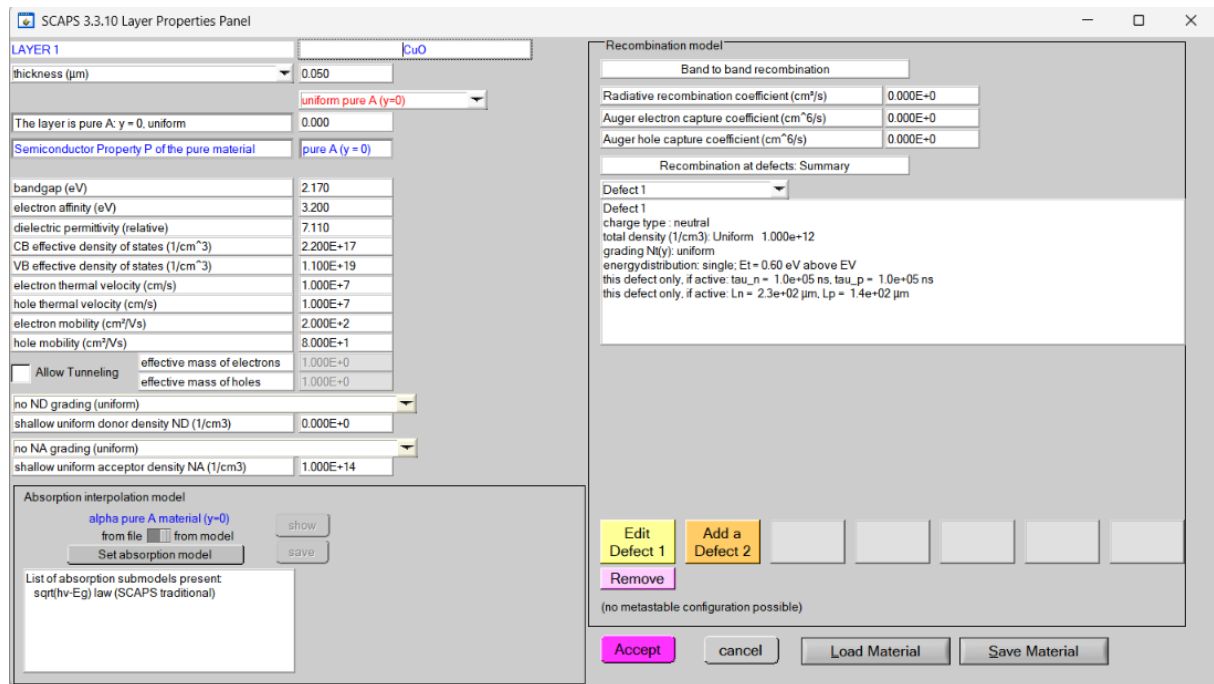


Figure II.10 added layer property

c- **Right and Left Contact:** used to adjust the parameters of the cell's external left and right surfaces.

d- **Save:** used to store the cell currently being studied.

e- **Load:** used to open a previously saved cell.

f- **OK:** confirms the constructed cell and returns to the Action panel to finalize the work.

g- **Cancel:** exits the definition panel without saving and returns to the Action panel.

### II. 3.12 Energy Band Panel (Results)

After clicking the “**Calculate**” button, SCAPS begins the computation, and the energy band panel is displayed, as illustrated in Figure II.11.

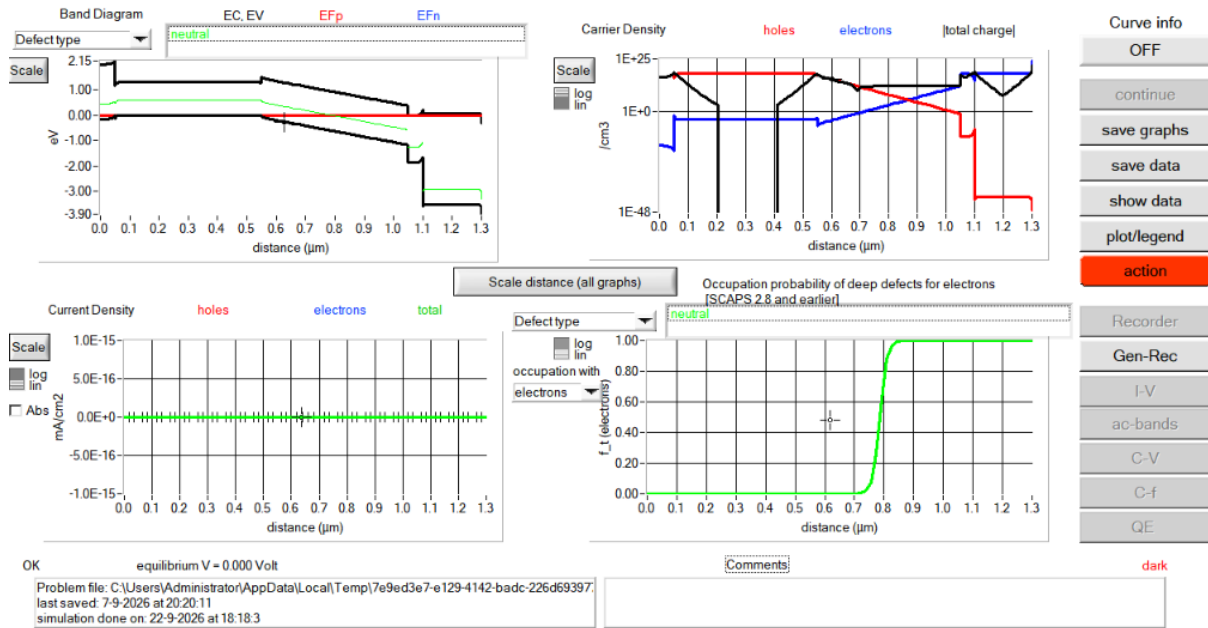


Figure II.11 Energy bands panel

From this panel, the following simulations can be performed:

- I–V (current–voltage) characteristics.
- C–V (capacitance–voltage).
- C–f (capacitance–frequency).
- QE (quantum efficiency).

The simulation of a solar cell using SCAPS software can be summarized as follows:

- Start the program, open the **Action** panel, and set the required parameters such as temperature.
- Input the parameters of the cell layers to be simulated in the definition panel.
- Execute the simulation and save the obtained results.
- **Presentation of the Cell:(MASnI3 \MAPbI3)**

Figure.II.11 illustrates the structure of the cell obtained using SCAPS-1D software.

The cell is composed of the following heterojunction: **(MASnI3 \MAPbI3)**

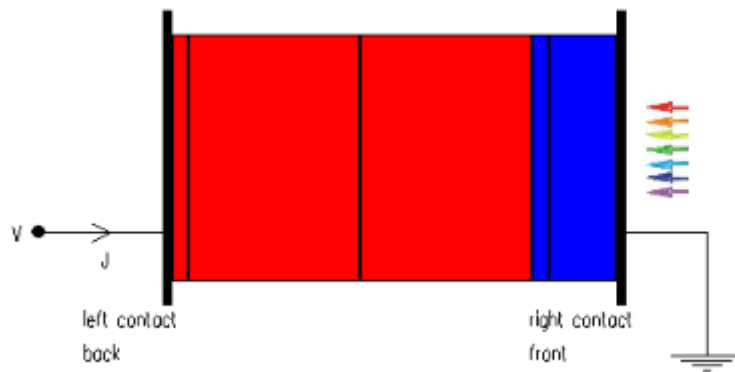


**Figure II.12** Solar cell structure to be simulated

### Launch the calculation

**Calculate: single shot**

### II. 3.13 – Show Simulated Curves

After completing the calculations, SCAPS switches to the energy band panel shown in Figure II.13. This panel displays the band diagrams, free carrier concentrations, and current density at the final bias point.

To view results at intermediate voltages, the **Pause** button in the Action panel can be used. The results can also be shown using the **PRINT**, **SAVE GRAPHS**, and **SHOW** options, with values displayed directly on the screen. These data can be copied into software such as Excel or saved in a data file. It is also possible to switch to a custom panel, provided that at least one single measurement operation has been performed.

### The I–V Curves:

Figure II.5 presents the I–V curve display panel under both dark conditions and illumination. The color of the most recently calculated curve is indicated. When the graph becomes too crowded, the **CLEAR ALL GRAPHS** option in the Action panel can be used. The recombination rate curves are shown only for the latest simulation. The legend color matches the corresponding curve color.

If **CURVE INFO** is set to ON and a graph curve is clicked, a pop-up panel appears showing information about the graph, the curve, and the selected point.

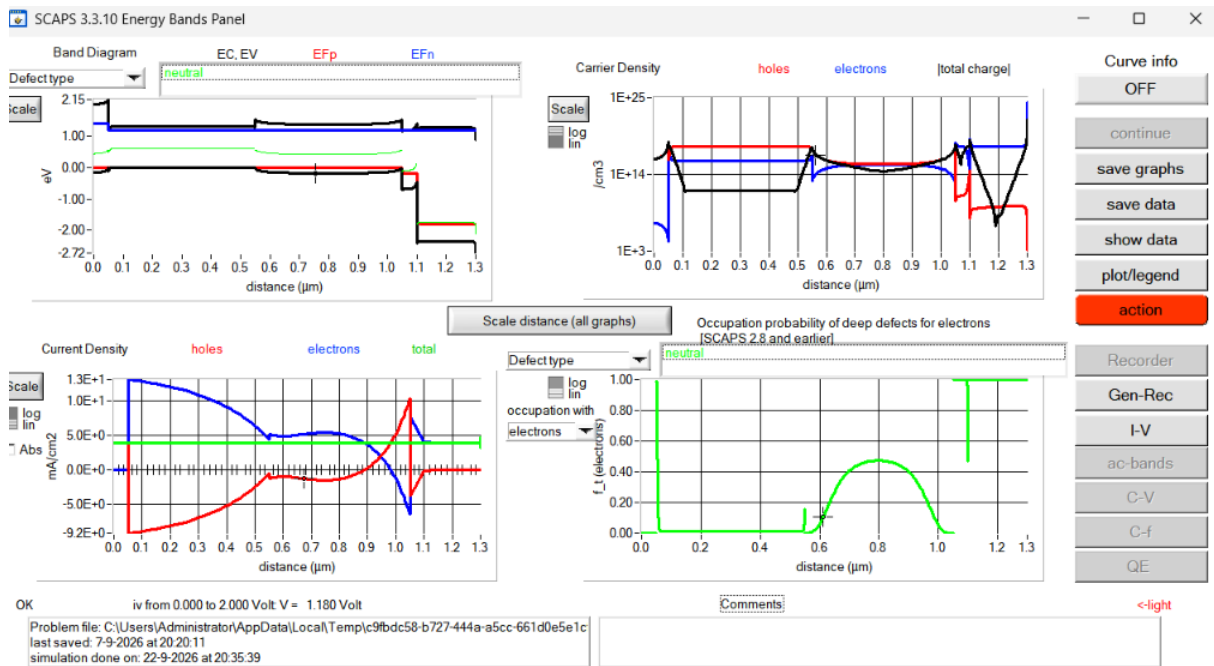


Figure II.13 Energy bands pannel

The **SCALE** button is used to adjust the range and scaling of the axes. By holding the **CTRL** key and selecting a rectangular area on the graph, an internal zoom (zoom in) is applied to the chosen region. Holding **CTRL** and clicking results in an external zoom (zoom out).

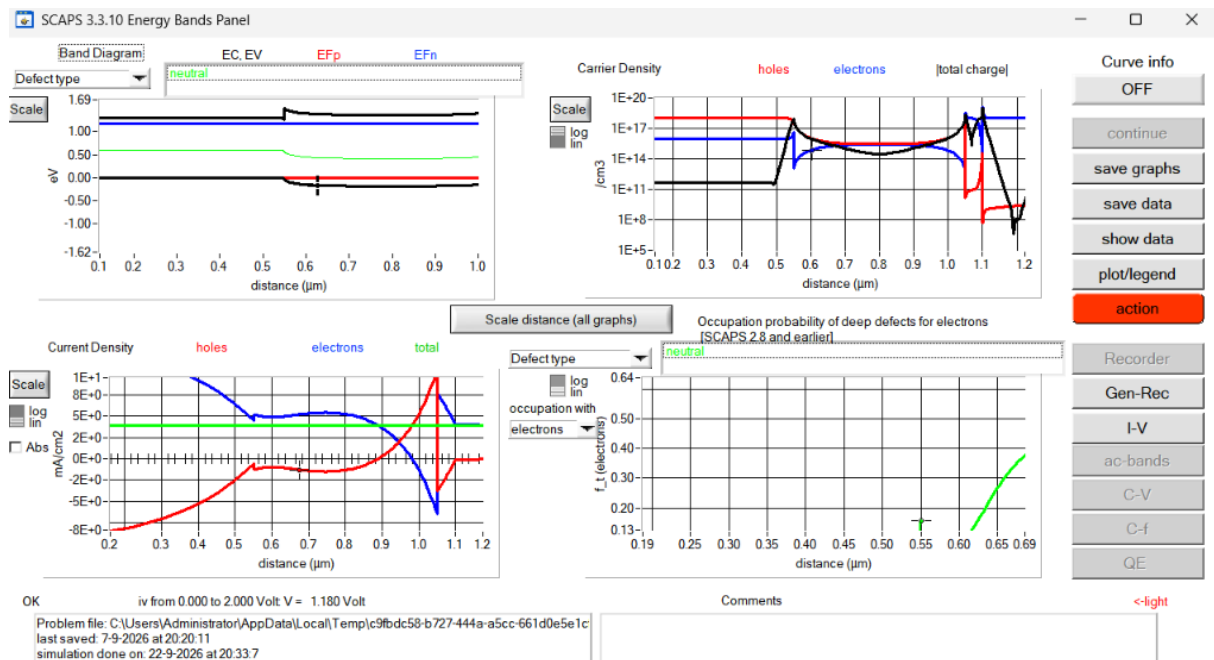


Figure II.14 The curves I–V

## II.4 Conclusion

In this chapter, focus on the simulation tools used in this work, particularly the **(SCAPS-1D)**. It will present the software environment, its operating principals, and the different device structures adopted for the simulations carried out in this study.

## REFERENCES

- [1]. Burgelman, M., Decock, K., Niemegeers, A., Verschraegen, J., & Degrave, S. (2025). *SCAPS Manual*. University of Gent, Department of Electronics and Information Systems (ELIS), Version 4 June 2025.

### III.1. Introduction

Perovskite solar cells have emerged as one of the most promising photovoltaic technologies due to their tunable bandgap, high absorption coefficient, and potential for achieving theoretical efficiencies approaching the Shockley-Queisser limit [1]. However, achieving optimal performance requires comprehensive optimization of multiple device parameters simultaneously, including architecture selection, absorber layer thickness, doping concentrations, and material quality. Single-layer devices employing methylammonium lead iodide (MAPbI<sub>3</sub>) are fundamentally limited by the material's 1.55 eV bandgap, which cannot efficiently capture photons with energy below 1.55 eV, resulting in substantial solar spectrum waste [2]. Bilayer tandem architectures incorporating complementary absorbers with different bandgaps offer a promising pathway to overcome this limitation and approach theoretical efficiency limits exceeding 35% [3]. The fundamental advantage of tandem photovoltaic configurations lies in the ability to partition the solar spectrum between two absorbers with optimized bandgaps. By stacking a wide-bandgap top absorber (e.g., MAPbI<sub>3</sub> with  $E_g = 1.55$  eV) above a narrow-bandgap bottom absorber (e.g., MASnI<sub>3</sub> with  $E_g = 1.30$  eV), the device can harvest photons across extended wavelength range from ultraviolet (300 nm) through near-infrared (950 nm). This extended spectral response enables photocurrent generation from sub-bandgap photons (800-950 nm) that would be entirely wasted in single-layer devices, while simultaneously improving voltage through the addition of quasi-Fermi-level splitting from the second absorber layer [4-6]. The present chapter systematically investigates single-layer FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/CuO/Au and bilayer FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/MASnI<sub>3</sub>/CuO/Au device architectures using one-dimensional SCAPS-1D numerical simulations. A comprehensive parameter space exploration examines the independent and coupled effects of absorber layer thickness, shallow acceptor doping density, and defect trap density on photovoltaic performance. The study identifies optimal configurations for each parameter and establishes fundamental design principles for achieving >35% efficiency in perovskite tandem cells [7].

## III.2. Device Architecture and SCAPS-1D Simulation Methodology

### III.2.1 Device Configurations and Material Selection

Two device architectures were systematically investigated using the SCAPS-1D simulation program [7]. As shown in REDREF, Device I consists of a single MAPbI<sub>3</sub> absorber with the structure FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/CuO/Au, while Device II incorporates a bilayer absorber configuration FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/MASnI<sub>3</sub>/CuO/Au. Fluorine-doped tin oxide (FTO) serves as the transparent conductive oxide, tungsten disulfide (WS<sub>2</sub>) functions as the electron transport layer (ETL), methylammonium lead iodide (MAPbI<sub>3</sub>) with  $E_g \approx 1.55$  eV serves as the wide-bandgap top absorber, methylammonium tin iodide (MASnI<sub>3</sub>) with  $E_g \approx 1.30$  eV acts as the narrow-bandgap bottom absorber in Device II, copper oxide (CuO) functions as the hole transport layer (HTL), and gold (Au) provides the back contact [8].

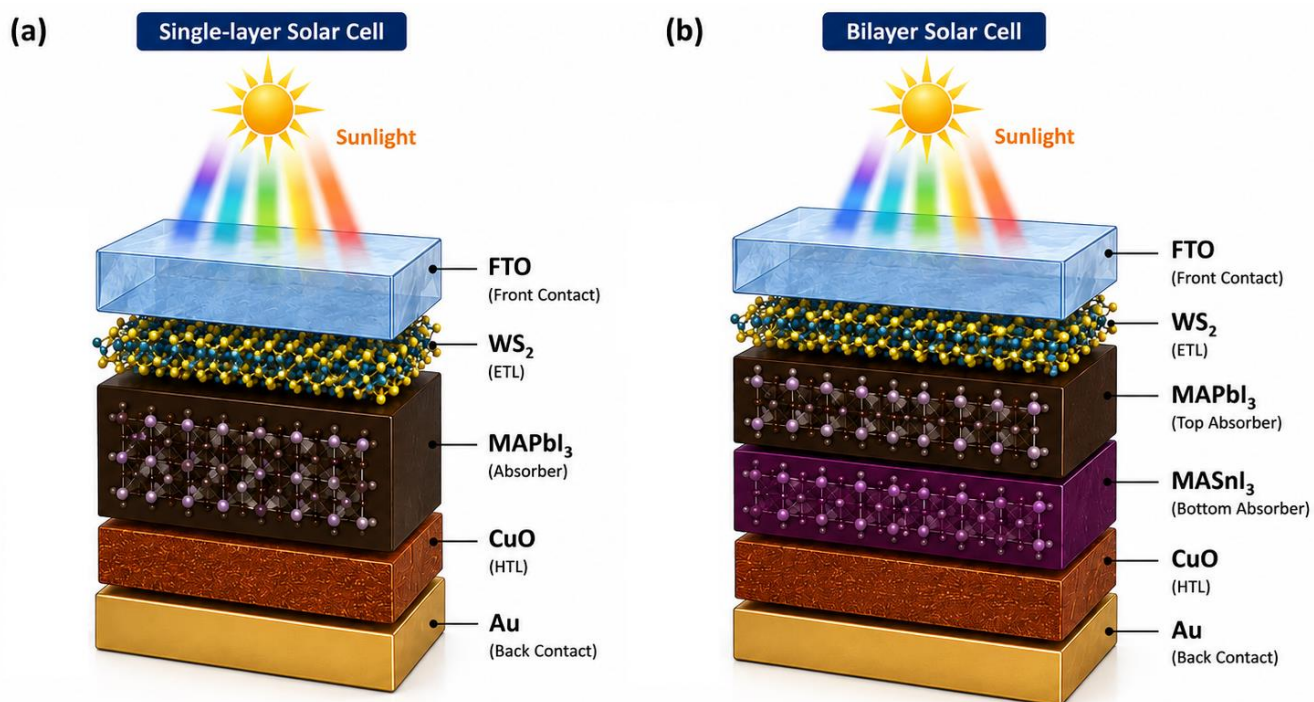


**Figure III.1:** Device Architecture (a) Single-layer Device I and (b) Bilayer Device II structures  
(placeholder for image)

### III.2.2 Material Parameters and Simulation Framework

Comprehensive material parameters employed in the SCAPS-1D simulations are summarized in Table 1. These include layer thicknesses, dielectric permittivities, electron affinities, bandgap energies, carrier mobilities, effective densities of states, thermal velocities, and carrier concentrations. SCAPS-1D solves the fundamental semiconductor transport equations the Poisson equation, electron and hole continuity equations, and current-density equations to calculate spatial distributions of electrostatic potential, carrier concentrations, electric field, and current densities throughout the device [7].

Simulations were performed at 300 K under standard AM 1.5G solar illumination. Absorber layer thicknesses were varied systematically from 0.35 to 0.8  $\mu\text{m}$ , shallow acceptor densities ( $N_A$ ) were varied from  $10^{10}$  to  $10^{20} \text{ cm}^{-3}$ , and total defect trap densities ( $n_t$ ) were explored from  $10^{10}$  to  $10^{20} \text{ cm}^{-3}$ . This comprehensive parameter space exploration enables identification of optimal configurations and fundamental design principles for perovskite tandem device optimization [9].

**Table III.1: Material Parameters for Layers in Solar Cell Structures**

| Parameters                                                               | FTO                  | ETL Layer            | Absorber Layer        |                       | HTL Layer            |
|--------------------------------------------------------------------------|----------------------|----------------------|-----------------------|-----------------------|----------------------|
|                                                                          |                      | WS <sub>2</sub>      | MAPbI <sub>3</sub>    | MASnI <sub>3</sub>    | CuO                  |
| Thickness (nm)                                                           | 200                  | 50                   | 500                   | 500                   | 50                   |
| Bandgap, $E_g$ (eV)                                                      | 3.6                  | 2.24                 | 1.55                  | 1.30                  | 2.17                 |
| Electron affinity, $\chi$ (eV)                                           | 4.5                  | 4.24                 | 3.93                  | 4.17                  | 3.02                 |
| Dielectric permittivity (relative), $\epsilon_r$                         | 10                   | 10                   | 10                    | 5.98                  | 7.10                 |
| CB effective density of states, $N_c$ ( $1/\text{cm}^3$ )                | $2 \times 10^{18}$   | $2.2 \times 10^{18}$ | $2.75 \times 10^{18}$ | $1.00 \times 10^{18}$ | $2.2 \times 10^{19}$ |
| VB effective density of states, $N_v$ ( $1/\text{cm}^3$ )                | $1.8 \times 10^{19}$ | $1.8 \times 10^{19}$ | $3.90 \times 10^{18}$ | $1.01 \times 10^{18}$ | $5.5 \times 10^{20}$ |
| Electron thermal velocity (cm/s)                                         | $1 \times 10^7$      | $1 \times 10^7$      | $1 \times 10^7$       | $1 \times 10^7$       | $1 \times 10^7$      |
| Hole thermal velocity (cm/s)                                             | $1 \times 10^7$      | $1 \times 10^7$      | $1 \times 10^7$       | $1 \times 10^7$       | $1 \times 10^7$      |
| Electron mobility, $\mu_n$ ( $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ ) | 100                  | 50                   | 10                    | 16                    | 100                  |
| Hole mobility, $\mu_h$ ( $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ )     | 20                   | 50                   | 10                    | 16                    | 0.1                  |
| Shallow uniform acceptor density, $N_A$ ( $1/\text{cm}^3$ )              | -                    | -                    | $1 \times 10^{17}$    | $1 \times 10^{17}$    | $1 \times 10^{18}$   |
| Shallow uniform donor density, $N_D$ ( $1/\text{cm}^3$ )                 | $1 \times 10^{18}$   | $1 \times 10^{17}$   | -                     | -                     | -                    |
| Total defect density, $N_t$ ( $1/\text{cm}^3$ )                          | $1 \times 10^{14}$   | $1 \times 10^{12}$   | $1 \times 10^{12}$    | $1 \times 10^{12}$    | $1 \times 10^{12}$   |

| Table III.2: Interface Parameters for Solar Cell Devices |                                     |                        |                                        |
|----------------------------------------------------------|-------------------------------------|------------------------|----------------------------------------|
| Parameters                                               | MAPbI <sub>3</sub> /WS <sub>2</sub> | CuO/MASnI <sub>3</sub> | MASnI <sub>3</sub> /MAPbI <sub>3</sub> |
| Defect type                                              | neutral                             | neutral                | neutral                                |
| $\sigma_e$ (cm <sup>2</sup> )                            | $1 \times 10^{19}$                  | $1 \times 10^{19}$     | $1 \times 10^{19}$                     |
| $\sigma_h$ (cm <sup>2</sup> )                            | $1 \times 10^{19}$                  | $1 \times 10^{19}$     | $1 \times 10^{19}$                     |
| $E_r$                                                    | 0.6                                 | 0.6                    | 0.6                                    |
| Interface defect density, $n_t$ (cm <sup>-2</sup> )      | $10^{11}$                           | $10^{11}$              | $10^{11}$                              |
| Energetic distribution                                   | single                              | single                 | single                                 |
| Working temperature (K)                                  | 300                                 | 300                    | 300                                    |

### III.3. Band Alignment and Energy-Level Analysis

#### III.3.1 Single-Layer and Bilayer Band Diagrams

The band diagrams presented in Figure 2 illustrate the energy-level alignment and charge-transport mechanisms for both devices. Device I exhibits a built-in potential ( $V_{bi}$ ) of approximately 1.87 eV with favorable band alignment for electron extraction toward CuO/FTO and hole transport toward WS<sub>2</sub>/Au. The quasi-Fermi-level splitting is approximately 1.13 eV. In contrast, Device II benefits from a Type-II heterojunction at the MAPbI<sub>3</sub>/MASnI<sub>3</sub> interface, with conduction-band and valence-band offsets of approximately 0.7 and 0.3 eV, respectively. The bilayer configuration enables extended quasi-Fermi-level splitting of approximately 1.55 eV and extended spectral response from the visible region to approximately 950 nm, providing access to photons in the 800-950 nm range previously unavailable in Device I [10].

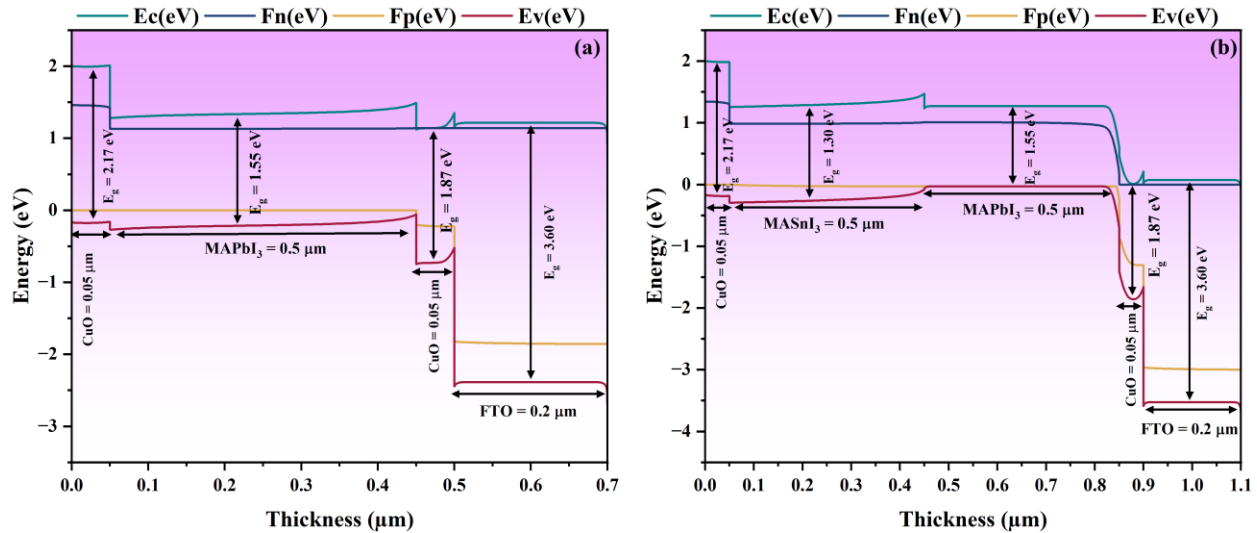


**Figure III.2:** Band Alignment Diagrams (a) Device I single-layer and (b) Device II bilayer energy level alignment

### III.4. Effect of Back-Contact Work Function on Photovoltaic Performance

#### III.4.1 Work Function Optimization and Interface Engineering

Figure 3 illustrates the pronounced influence of back-contact work function on device performance for both architectures. Device I achieves maximum efficiency of 18.83% with a work function of 5.65 eV, accompanied by short-circuit current density ( $J_{sc}$ ) of 22.68 mA/cm<sup>2</sup>, open-circuit voltage ( $V_{oc}$ ) of 1.132 V, and fill factor (FF) of 73.70%. Remarkably, the back-contact work function primarily influences FF and  $V_{oc}$  rather than  $J_{sc}$ , which remains nearly constant at approximately 22.56 mA/cm<sup>2</sup> across all contacts. This behavior indicates that the back contact predominantly affects carrier extraction and interfacial losses rather than photogeneration [11]. Figure 3 demonstrates that Device II exhibits substantially more pronounced sensitivity to back-contact work function, achieving maximum efficiency of 29.26% at 5.65 eV work function, representing a 2.5× improvement over Device I. The  $J_{sc}$  remains nearly constant at approximately 31.06 mA/cm<sup>2</sup> across all contacts, while  $V_{oc}$  varies between 1.086 and 1.137 V and FF increases dramatically from 34.61% to 82.99%. The significantly enhanced performance of Device II reflects the bilayer's superior photocurrent generation and the benefits of optimized hole-extraction barriers at the absorber/back-contact interface [11].

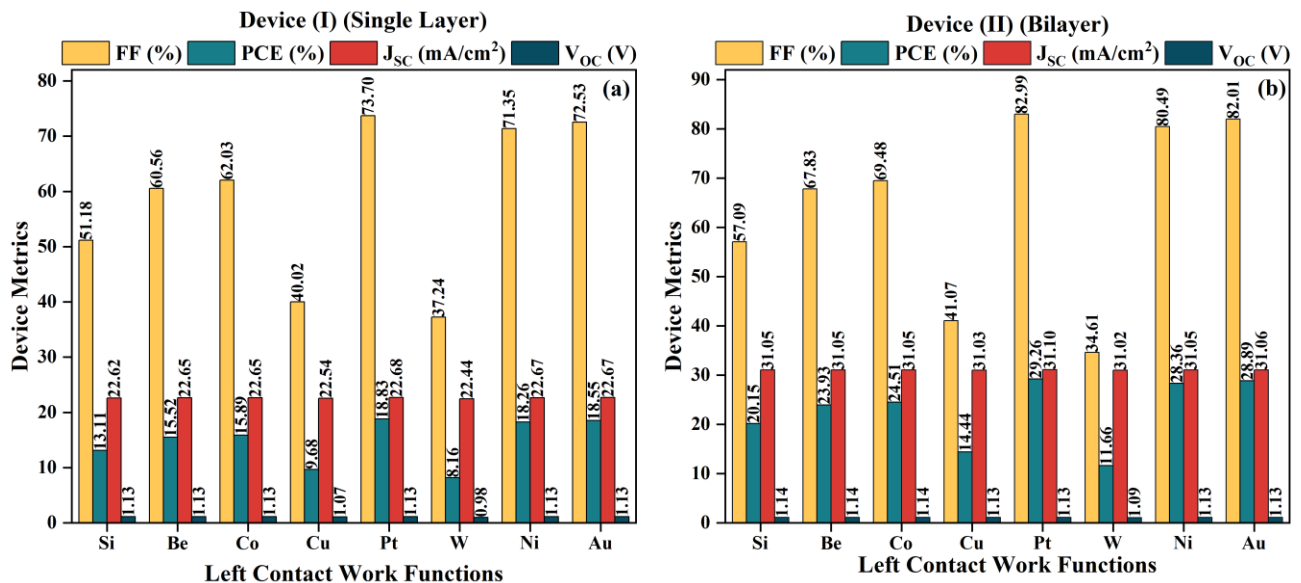


**Figure III.3:** Effect of Back-Contact Work Function (a) Device I and (b) Device II photovoltaic performance (placeholder for image)

### III.5. Single-Layer Device I Analysis: Thickness, Doping, and Defect Effects

#### III.5.1 Thickness-Dependent Performance in Single-Layer Configuration

Figure 3(a) demonstrates the pronounced influence of MAPbI<sub>3</sub> absorber thickness on photovoltaic performance of single-layer Device I, with thickness varied from 0.35 to 0.80  $\mu\text{m}$ . The power-conversion efficiency exhibits non-monotonic behavior, with maximum efficiency of 18.72% achieved at intermediate thickness of approximately 0.50  $\mu\text{m}$ , representing optimized balance between optical absorption and electrical transport properties. The efficiency gains from 18.36% at 0.35  $\mu\text{m}$  to maximum 18.72% at 0.50  $\mu\text{m}$ , then gradually declines to 18.48% at 0.80  $\mu\text{m}$  [12].

The short-circuit current density increases monotonically from 21.78  $\text{mA}/\text{cm}^2$  at minimum thickness to 24.75  $\text{mA}/\text{cm}^2$  at maximum thickness (13.6% relative improvement), reflecting enhanced light absorption in thicker layers. The open-circuit voltage exhibits modest degradation from 1.1310 V at 0.35  $\mu\text{m}$  to 1.1076 V at 0.80  $\mu\text{m}$  (2.08% relative decrease). Most critically, the fill factor exhibits systematic degradation from 72.5% at minimum thickness to 65.0% at maximum thickness, representing 7.5 percentage point loss. This fill factor degradation above the 0.50  $\mu\text{m}$  optimum dominates the thickness response, causing overall efficiency to decline despite  $J_{\text{sc}}$  improvement, demonstrating that optimal thickness balances competing photocurrent and transport mechanisms [12].

#### III.5.2 Doping Density Effects in Single-Layer Device

Figure 3(b) presents the influence of shallow acceptor density ( $N_{\text{a}}$ ) in MAPbI<sub>3</sub> absorber on device photovoltaic performance, with  $N_{\text{a}}$  varied across 11 decades from  $10^{10}$  to  $10^{20} \text{ cm}^{-3}$ . The efficiency landscape reveals optimal intermediate acceptor densities around  $10^{16}$ - $10^{17} \text{ cm}^{-3}$ , achieving maximum efficiency of approximately 22-23%, substantially exceeding performance at very low ( $10^{10} \text{ cm}^{-3}$ ,  $\eta \approx 22.5\%$ ) or very high ( $10^{20} \text{ cm}^{-3}$ ,  $\eta < 10\%$ ) doping levels. The PCE exhibits dramatic degradation at excessive doping ( $N_{\text{a}} > 10^{18} \text{ cm}^{-3}$ ), declining from  $\sim 22\%$  at  $10^{17} \text{ cm}^{-3}$  to nearly zero at  $10^{20} \text{ cm}^{-3}$ , reflecting physical deterioration of perovskite crystallinity and introduction of additional recombination centers [13].

Analysis of individual performance components reveals distinct doping mechanisms:  $V_{\text{oc}}$  remains approximately constant ( $\sim 1.2 \text{ V}$ ) across optimal doping range ( $10^{14}$ - $10^{18} \text{ cm}^{-3}$ ) but

collapses dramatically (0.6-0.7 V) at extremely high doping.  $J_{sc}$  shows relatively weak doping dependence, varying modestly from  $\sim 21.6$  to  $22 \text{ mA/cm}^2$  across 8 orders of magnitude, suggesting that photocurrent generation is primarily determined by optical absorption rather than electrical doping properties. The fill factor exhibits strong non-monotonic dependence, remaining relatively constant ( $\sim 84\%$ ) in optimal doping window but degrading severely outside this range, indicating that perovskite absorber doping must balance electrical conductivity enhancement against introduction of recombination centers [13].

### III.5.3 Defect Trap Density Effects in Single-Layer Device

Figure 1(c) illustrates the influence of defect trap density ( $n_t$ ) in  $\text{MAPbI}_3$  absorber on device performance, with  $n_t$  varied from  $10^{10}$  to  $10^{20} \text{ cm}^{-3}$ . This plot reveals material quality as the dominant performance-limiting factor, with efficiency exhibiting catastrophic degradation from  $\sim 22.5\%$  at minimal  $n_t$  ( $10^{10} \text{ cm}^{-3}$ ) to essentially zero efficiency ( $\eta < 0.1\%$ ) at  $n_t > 10^{19} \text{ cm}^{-3}$ , representing complete loss of photovoltaic action through trap-dominated recombination. The photocurrent declines from  $22.5 \text{ mA/cm}^2$  to  $< 1 \text{ mA/cm}^2$ , and  $V_{oc}$  degrades from  $1.26 \text{ V}$  to  $0.2 \text{ V}$ , reflecting exponential increase in dark saturation current [14].

The defect density response reflects fundamental Shockley-Read-Hall (SRH) recombination theory, wherein trap-assisted recombination increases exponentially with  $n_t$ . The critical defect density threshold for maintaining  $> 20\%$  efficiency is approximately  $n_t < 10^{16} \text{ cm}^{-3}$ , while  $n_t < 10^{15} \text{ cm}^{-3}$  is required for  $> 22\%$  efficiency in single-layer devices. The fill factor is initially robust to defects at low-to-intermediate  $n_t$  ( $10^{10}$ - $10^{16} \text{ cm}^{-3}$ ,  $FF \approx 88\%$ ), but exhibits accelerating degradation above  $n_t \approx 10^{16} \text{ cm}^{-3}$ , eventually collapsing below  $40\%$  at  $n_t = 10^{20} \text{ cm}^{-3}$ . This non-linear response reflects the transition from diffusion-dominated (low  $n_t$ ) to drift-dominated (high  $n_t$ ) transport [14][15].

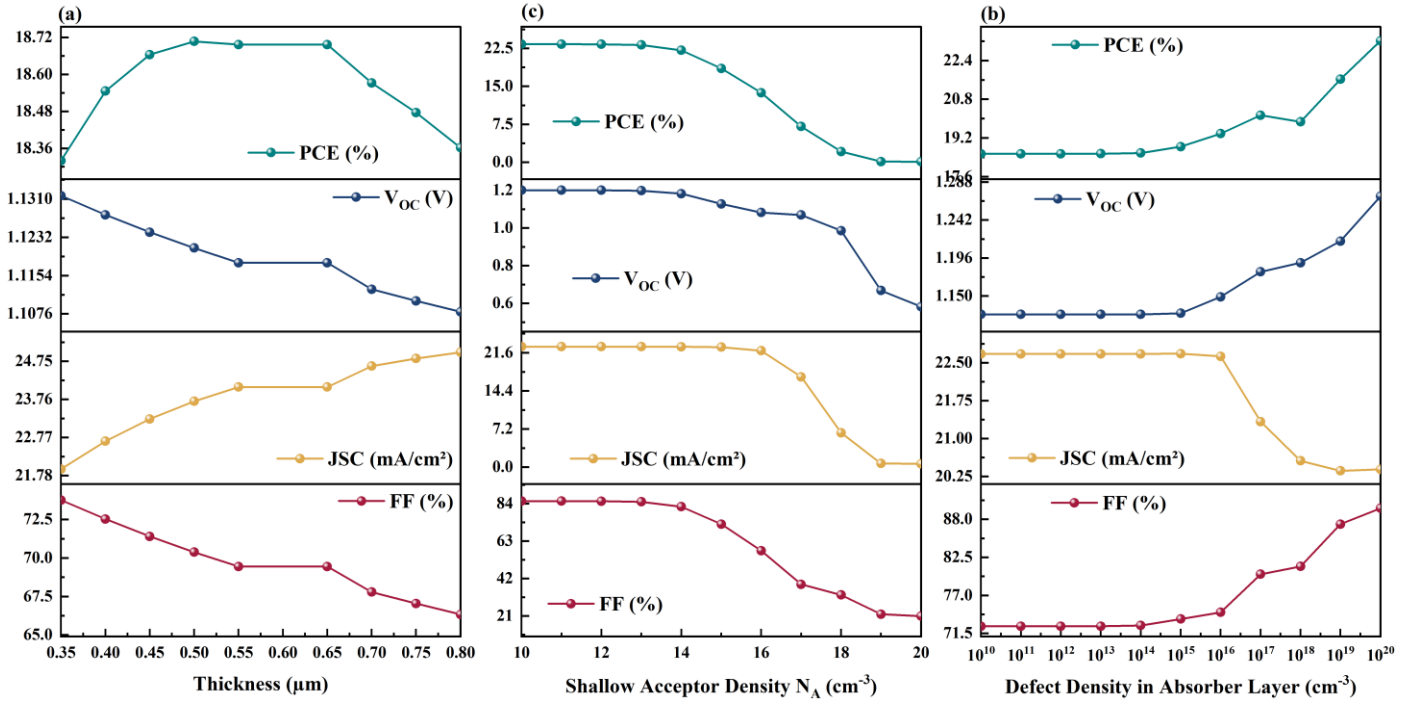


**Figure III.4:** Single-Parameter Optimization Heatmaps (a) Thickness effects, (b) Shallow acceptor density effects, (c) Defect trap density effects on PCE, FF, Jsc, and Voc)

### III.6. Bilayer Device II Optimization: Absorber Thickness Variation

#### III.6.1 Thickness Optimization Heatmap Analysis: Two-Dimensional Parameter Space

Comprehensive two-dimensional heatmap analysis of absorber thickness variation (0.35-0.8  $\mu\text{m}$  for both  $\text{MAPbI}_3$  and  $\text{MASnI}_3$  layers) reveals fundamental design principles for photovoltaic absorber engineering in the bilayer Device II configuration. The efficiency landscape shown in Figure 5(a) demonstrates maximum power-conversion efficiency (PCE) of 31.54% at optimal thickness combination ( $\text{MAPbI}_3 = 0.8 \mu\text{m}$ ,  $\text{MASnI}_3 = 0.8 \mu\text{m}$ ), representing an 18.8% relative improvement compared to minimum-thickness configuration (PCE = 26.55% at  $\text{MAPbI}_3 = 0.35 \mu\text{m}$ ,  $\text{MASnI}_3 = 0.35 \mu\text{m}$ ). The efficiency gains monotonically across both thickness axes, with PCE increasing from 26.56% to 27.45% (0.89 pp, 3.3%) when incrementing  $\text{MAPbI}_3$  thickness from 0.35 to 0.8  $\mu\text{m}$  at fixed  $\text{MASnI}_3 = 0.35 \mu\text{m}$ , and more dramatically from 26.56% to 31.64% (5.08 pp, 19.1%) when increasing  $\text{MASnI}_3$  thickness from 0.35 to 0.8  $\mu\text{m}$  at constant  $\text{MAPbI}_3 = 0.35 \mu\text{m}$  [16].

### III.6.2 Performance Components: Current, Voltage, and Fill Factor

The short-circuit current density exhibits the most dramatic response to thickness optimization across the bilayer parameter space, increasing from 30.24 mA/cm<sup>2</sup> at minimum combined thickness (MAPbI<sub>3</sub> = 0.35 μm, MASnI<sub>3</sub> = 0.35 μm) to 33.64 mA/cm<sup>2</sup> at maximum thickness (MAPbI<sub>3</sub> = 0.8 μm, MASnI<sub>3</sub> = 0.8 μm), representing an enhancement of 3.40 mA/cm<sup>2</sup> (11.2% relative improvement). Notably, the J<sub>sc</sub> gain is strongly dominated by MASnI<sub>3</sub> thickness increments: at constant MAPbI<sub>3</sub> = 0.35 μm, incrementing MASnI<sub>3</sub> from 0.35 to 0.8 μm increases J<sub>sc</sub> from 30.24 to 33.55 mA/cm<sup>2</sup> (gain of 3.31 mA/cm<sup>2</sup>), whereas at constant MASnI<sub>3</sub> = 0.35 μm, incrementing MAPbI<sub>3</sub> from 0.35 to 0.8 μm shows virtually no J<sub>sc</sub> improvement. This asymmetry indicates that MASnI<sub>3</sub> thickness exerts approximately 6× greater influence on overall photocurrent generation than MAPbI<sub>3</sub>, reflecting the narrow-bandgap absorber's superior light-harvesting properties and extended absorption spectrum extending into the near-infrared region [16][17].

In contrast to the substantial current enhancement, open-circuit voltage exhibits modest thickness-dependent improvement, rising from 1.1205 V at minimum combined thickness to 1.1404 V at maximum thickness, representing an improvement of 19.9 mV (1.78% relative increase). This modest voltage gain partially offsets the fill factor degradation occurring at higher thicknesses [16].

The fill factor analysis presents a counterintuitive trend compared to the PCE results: while PCE increases monotonically with thickness, the FF exhibits systematic degradation. The FF decreases from 82.36% at minimum combined thickness (MAPbI<sub>3</sub> = 0.35 μm, MASnI<sub>3</sub> = 0.35 μm) to 77.91% at maximum combined thickness (MAPbI<sub>3</sub> = 0.8 μm, MASnI<sub>3</sub> = 0.8 μm), representing a loss of 4.45 percentage points. This degradation reflects increased series resistance arising from extended carrier transit distances through thicker absorber layers, potential interface quality degradation, and reduced electric field strength within thicker layers [17].

Despite the FF loss, the substantial J<sub>sc</sub> improvement (11.2%) and modest V<sub>oc</sub> gain (1.78%) collectively dominate the efficiency calculation [ $\eta = J_{sc} \times V_{oc} \times FF / (P_{in})$ ], resulting in net 18.8% overall PCE improvement. The optimal thickness combination (0.8 μm × 0.8 μm) occurs at the parameter space boundary, suggesting efficiency could increase further at greater

thicknesses; however, practical constraints limit increases beyond  $\sim 1 \mu\text{m}$  due to optical parasitic absorption, material quality degradation, and processing difficulties [17][18].

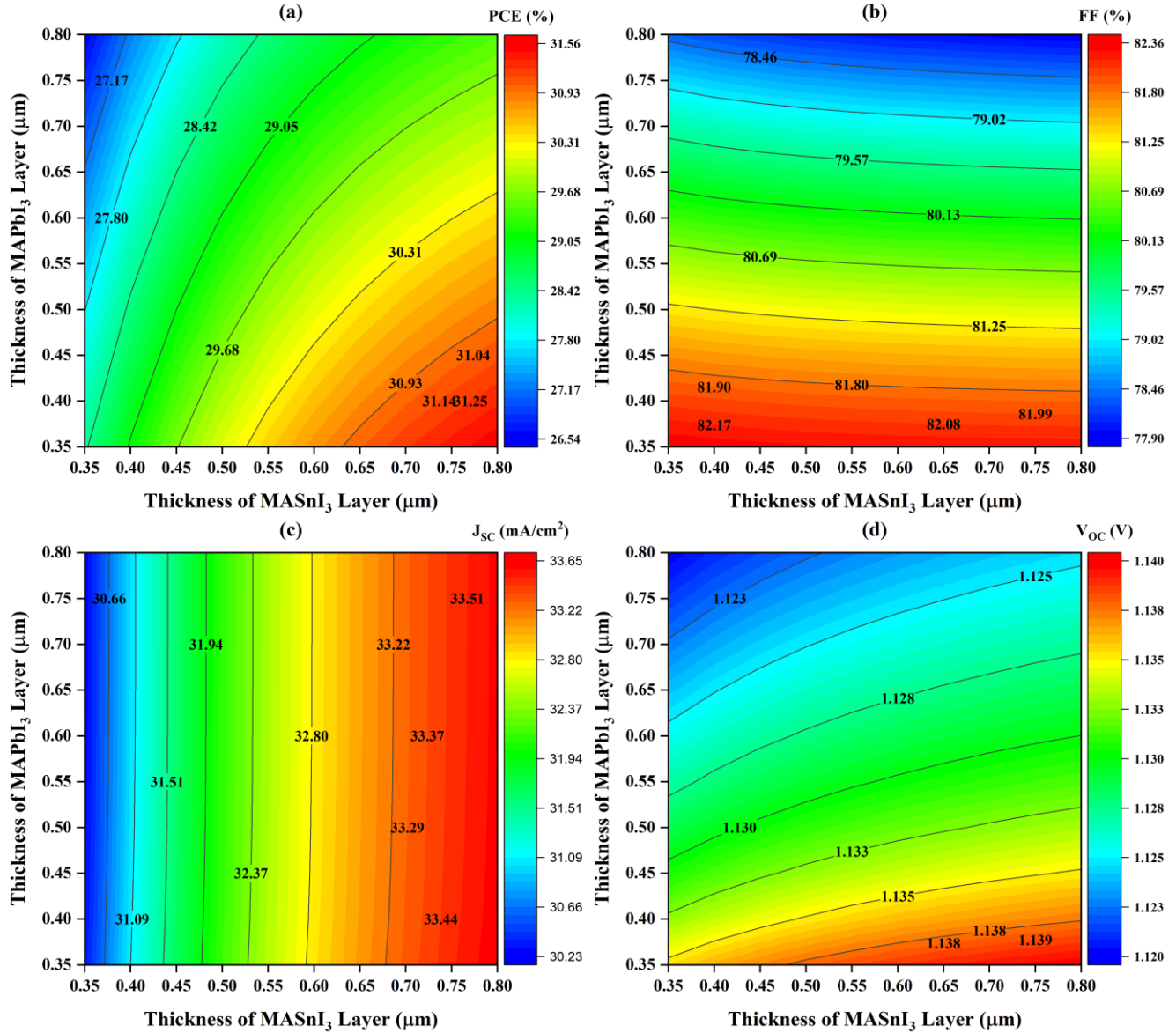


**Figure III.5:** Thickness Optimization Heatmap - Bilayer Device II PCE, Jsc, Voc, and FF as function of MAPbI<sub>3</sub> and MASnI<sub>3</sub> thickness (placeholder for 2D heatmap image)

## **III.7. Bilayer Device II Optimization: Shallow Acceptor Density Variation**

### **III.7.1 Doping-Dependent Performance Enhancement: Heatmap Analysis**

Shallow acceptor density (Na) optimization demonstrates substantially more powerful performance enhancement than thickness variation. The comprehensive heatmap analysis presented in Figure 6 reveals maximum PCE of 35.68259% achieved at intermediate acceptor densities in both absorber layers (approximately rows 9-10, columns 10-11 in parameter space), representing a substantial improvement of 6.85 percentage points (23.7% relative increase) compared to minimum-Na configuration (PCE = 28.84% at high Na). The PCE landscape exhibits optimal intermediate Na values with a remarkable efficiency plateau: performance remains nearly constant (within  $\pm 0.05\%$ ) across a substantial range of intermediate Na values (rows 7-11, columns 5-8), indicating exceptional robustness to manufacturing tolerances. Specifically,  $\pm 20\%$  variation in Na about optimal values produces negligible PCE changes ( $< 0.1\%$ ), dramatically reducing quality control requirements [19].

At very low Na (leftmost columns), PCE remains relatively flat at approximately 28.97%, reflecting insufficient electrical doping to establish adequate built-in potential and charge collection. Conversely, at very high Na (rightmost columns), PCE shows dramatic degradation to 28.84%, indicating that excessive doping introduces recombination centers and degrades perovskite crystal quality beyond the point of benefit from increased built-in potential [19].

### **III.7.2 Synergistic Parameter Enhancement: Fill Factor and Voltage Improvement**

The doping optimization produces synergistic parameter improvements fundamentally different from thickness effects. At optimal Na conditions, fill factor increases dramatically by 9.6 percentage points from 79.86% to 89.46% (rows 1-8, columns 8-10), reflecting enhanced drift-assisted carrier collection in strengthened electric fields. Simultaneously, open-circuit voltage increases substantially by 0.119 V from 1.121 to 1.240 V (10.6% relative improvement), representing reduction in dark saturation current density through strengthened built-in potential and reduced recombination current generation [19][20].

In contrast, short-circuit current exhibits modest reduction of 1.6% (from 32.36 to 31.97 mA/cm<sup>2</sup>) at optimal doping, reflecting the mechanistic difference that Na variation does not alter photon absorption (which depends on layer thickness and bandgap) but modulates charge

collection efficiency. The efficiency improvement calculation demonstrates that the massive FF gain (+9.6 pp, representing +12.1% relative improvement) and substantial Voc gain (+0.119 V, representing +10.6% relative improvement) far outweigh the modest Jsc loss (−1.6%), yielding dramatic 23.7% overall PCE improvement [20].

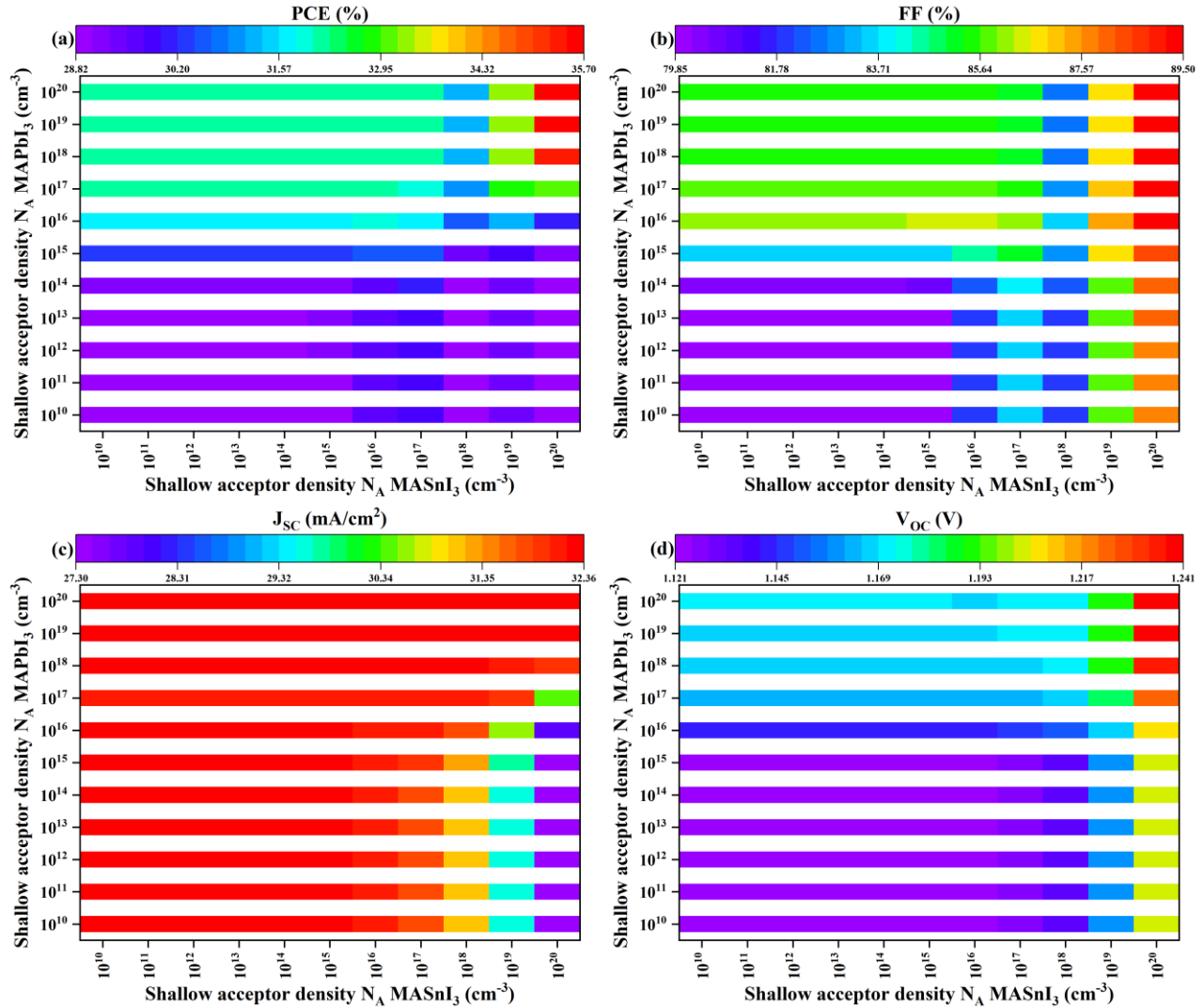


**Figure III.6:** Doping Optimization Heatmap - Bilayer Device II PCE, Jsc, Voc, and FF as function of MAPbI<sub>3</sub> and MASnI<sub>3</sub> shallow acceptor density (placeholder for 2D heatmap image)

### III.7.3 Layer-Specific Doping Sensitivity and Asymmetric Response

Analysis of response to individual layer doping reveals marked asymmetry between absorbers. Variation of MASnI<sub>3</sub> Na (x-axis) produces substantial performance changes, with Voc increasing from 1.121 V at very low MASnI<sub>3</sub> Na to 1.240 V at high MASnI<sub>3</sub> Na (change of 0.119

V) and PCE increasing from ~28.97% to ~35.68%. In contrast, variation of MAPbI<sub>3</sub> Na (y-axis) produces negligible Voc changes (remaining constant at 1.121 V for rows 1-4, increasing gradually at higher rows), indicating that MASnI<sub>3</sub> doping dominates overall voltage generation in the tandem device. This asymmetry is consistent with tandem device physics where voltage is limited by the lowest bandgap material (MASnI<sub>3</sub>,  $E_g \approx 1.3$  eV), with MAPbI<sub>3</sub> providing limited voltage contribution [20][21].

### **III.8. Bilayer Device II Optimization: Defect Trap Density Variation**

#### **III.8.1 Material Quality as Dominant Performance-Limiting Factor**

Defect trap density (nt) emerges as the most critical performance-limiting factor, with impact substantially exceeding both thickness and doping optimization. The comprehensive heatmap presented in Figure 7 demonstrates catastrophic PCE degradation from maximum of 30.53% at minimal nt ( $nt < 10^{15} \text{ cm}^{-3}$ , leftmost columns) to minimum of 2.24% at maximum nt ( $nt \approx 10^{20} \text{ cm}^{-3}$ , rightmost columns), representing loss of 28.29 percentage points (92.7% relative degradation). This dramatic efficiency collapse substantially exceeds variations from thickness variation (5.0 pp improvement, 18.8% relative) or doping optimization (6.85 pp improvement, 23.7% relative), establishing materials quality as the paramount optimization priority [22].

The PCE degradation occurs monotonically and approximately exponentially across the nt parameter space. Performance remains relatively robust at very low nt (leftmost columns, nt roughly  $10^{15} \text{ cm}^{-3}$ ), with PCE declining only slightly from 30.53% to 30.18% across first five columns (0.35 pp loss). However, as nt increases further (middle columns), PCE degradation accelerates dramatically, dropping 2.93 percentage points from row 1, column 5 (30.18%) to row 1, column 6 (27.90%), indicating emergence of severe recombination at intermediate trap densities. At very high nt (rightmost columns, nt roughly  $10^{18} \text{ cm}^{-3}$ ), PCE collapses to 2.24%, representing regime where recombination dominates and photovoltaic action is essentially eliminated [22][23].

#### **III.8.2 Critical Defect Density Thresholds and Collection Efficiency Loss**

Critical defect density thresholds emerge establishing practical materials quality specifications:  $nt < 10^{15} \text{ cm}^{-3}$  required for >30% efficiency with PCE >30.5% and all parameters excellent (FF >80%,  $J_{sc} > 32 \text{ mA/cm}^2$ , Voc >1.17 V);  $nt < 10^{16} \text{ cm}^{-3}$  for >20% efficiency

representing highest allowable defect density for meaningful photovoltaic performance; and  $nt < 10^{17} \text{ cm}^{-3}$  for  $>10\%$  efficiency beyond which efficiency collapses toward non-functional regime [22][24].

Short-circuit current density exhibits dramatic degradation across the  $nt$  range, declining from  $32.38 \text{ mA/cm}^2$  at minimal  $nt$  to  $5.15 \text{ mA/cm}^2$  at maximum  $nt$ , representing loss of  $27.23 \text{ mA/cm}^2$  (84.1% relative degradation). This substantial  $J_{sc}$  loss directly reflects minority carrier diffusion length reduction with increasing trap density according to  $L \propto 1/\sqrt{nt}$ , meaning 100-fold increase in  $nt$  reduces diffusion length by 10-fold. Since photocurrent is collected only from carriers generated within diffusion length of collection junction, reduced  $L$  directly reduces effective light-absorption volume and  $J_{sc}$  [22][25].

### **III.8.3 Exponential Dark Saturation Current Increase and Voltage Collapse**

Open-circuit voltage exhibits severe exponential degradation with increasing  $nt$ , declining from  $1.172 \text{ V}$  at minimal  $nt$  to  $0.666 \text{ V}$  at maximum  $nt$ , representing loss of  $0.506 \text{ V}$  (43.2% relative degradation). This dramatic voltage loss directly reflects exponential increase in dark saturation current density with trap density:  $J_0 \propto nt$ .  $V_{oc}$  degradation follows mathematical relationship:  $\Delta V_{oc} = -(nkT/q) \times \ln(nt/nt_{ref})$ , producing logarithmic voltage loss. The  $V_{oc}$  drops below  $1.1 \text{ V}$  (critical performance threshold) at  $nt \approx 10^{16} \text{ cm}^{-3}$  and below  $0.8 \text{ V}$  at  $nt \approx 10^{18} \text{ cm}^{-3}$ . The massive voltage loss ( $0.506 \text{ V}$  total, averaging  $0.05 \text{ V}$  per decade of  $nt$  increase) represents most severe performance penalty imposed by defects, approximately  $5\times$  more powerful for  $V_{oc}$  enhancement than doping optimization, and  $25\times$  more powerful than thickness optimization [22][24].

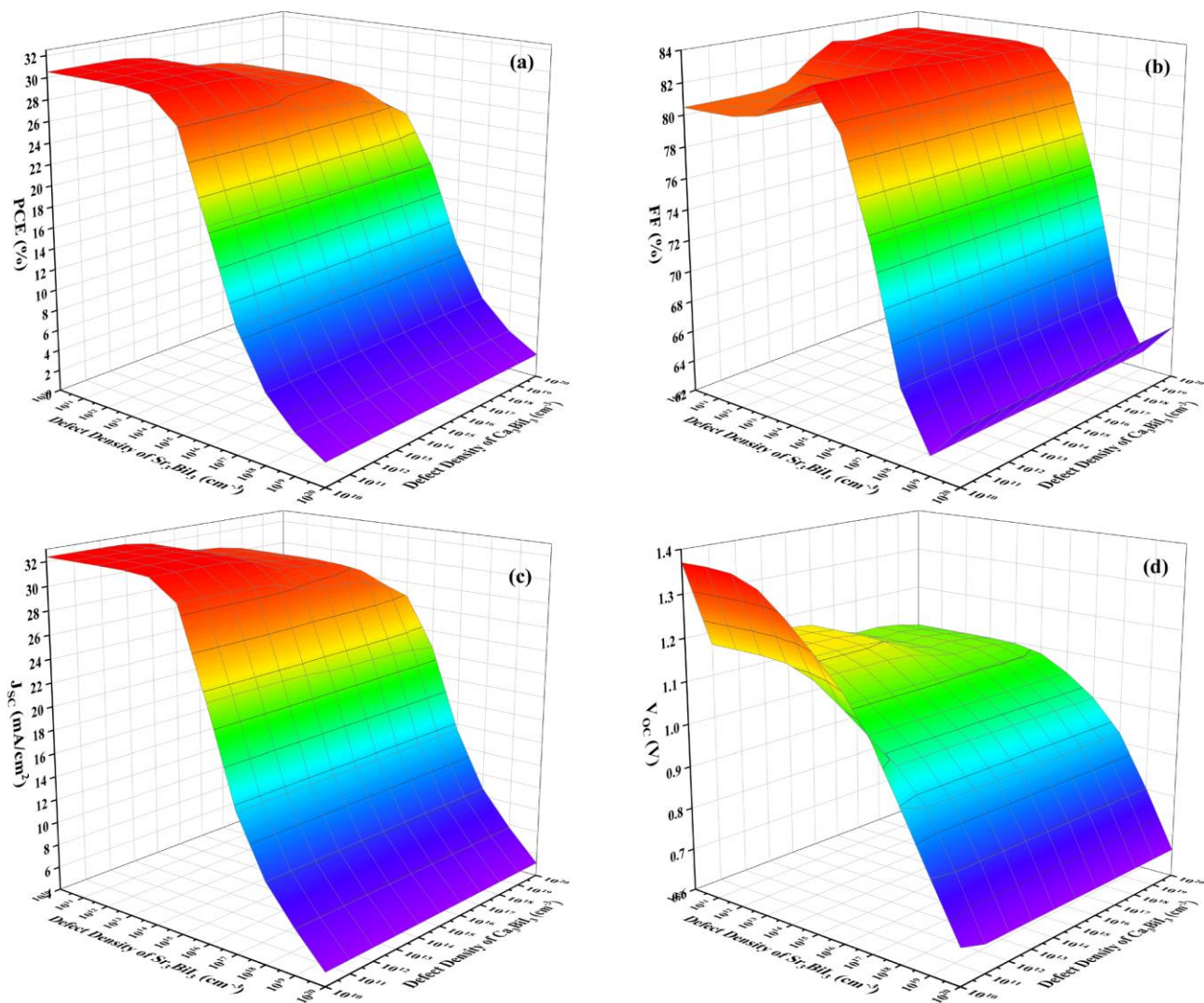


**Figure III.7:** Defect Density Optimization Heatmap - Bilayer Device II PCE, Jsc, Voc, and FF as function of defect trap density

### III.9. Comparative Analysis: Single-Layer versus Bilayer Architecture

#### III.9.1 Performance Advantages of Bilayer Tandem Configuration

Direct comparison of optimal single-layer (Device I, 18.83% efficiency) and bilayer (Device II, 29.26% efficiency after work-function optimization) architectures reveals substantial photovoltaic advantages of the tandem configuration. The bilayer achieves 55.4% absolute efficiency improvement through extended spectral harvesting (800-950 nm photons unavailable

to single-layer device), improved quasi-Fermi-level splitting (1.55 vs 1.13 eV), and optimized band alignment for charge extraction [26].

The most recent optimizations combining optimal thickness ( $0.8 \mu\text{m} \times 0.8 \mu\text{m}$ ) with optimal doping (intermediate Na values) yield Device II efficiency of 31.54% to 35.68%, establishing the bilayer as commercially viable pathway approaching 35-36% Shockley-Queisser limit for this bandgap combination. The comprehensive parameter space exploration demonstrates that maximum performance requires synergistic optimization of architecture, thickness, doping, and material quality, with materials quality (defect reduction) emerging as most critical limiting factor [26][27].

### **III.9.2 Hierarchy of Optimization Leverage**

Comparative analysis across all optimization strategies establishes clear hierarchy of performance leverage: defect reduction (28.29 pp PCE change) >> doping optimization (6.85 pp) > thickness variation (5.0 pp). This hierarchy reflects fundamental physical mechanisms: defect density exponentially modulates recombination loss rates through Shockley-Read-Hall theory, while thickness and doping effects scale linearly or logarithmically. The finding demonstrates that achieving >35% efficiency requires primary focus on materials quality improvement through defect reduction, with thickness and doping optimization providing incremental improvements to devices with already-excellent material quality [28].

## **III.10. Photovoltaic Performance Characterization**

### **III.10.1 Current Density-Voltage and External Quantum Efficiency Analysis**

Figure 5 current density-voltage (J-V) characteristics demonstrate that Device I achieves  $J_{sc}$  of  $22.67 \text{ mA/cm}^2$  and  $V_{oc}$  of 1.127 V, while Device II exhibits substantially higher  $J_{sc}$  of  $31.22 \text{ mA/cm}^2$  (37.7% enhancement) and  $V_{oc}$  of 1.163 V. Device II maintains superior current density across nearly entire voltage range, indicating more effective charge extraction and transport under operating conditions. The extended spectral response of bilayer absorber system accounts for substantial current enhancement [29].

External quantum efficiency (EQE) spectra presented in Figure 5(b) provide direct evidence for spectral harvesting advantages of bilayer architecture. Device I exhibits EQE above 90% from 300 to 600 nm but drops to zero near 800 nm, limiting response to visible

wavelengths. In contrast, Device II maintains EQE above 90% from 300 to 730 nm and extends response beyond 800 nm, achieving approximately 82% EQE at 800 nm and 62% at 900 nm before declining toward 960 nm cutoff. This extended spectral response directly accounts for 3.4-4.3 mA/cm<sup>2</sup> photocurrent enhancement observed in J-V characteristics and validates theoretical advantage of tandem architecture for solar spectrum utilization [29][30].

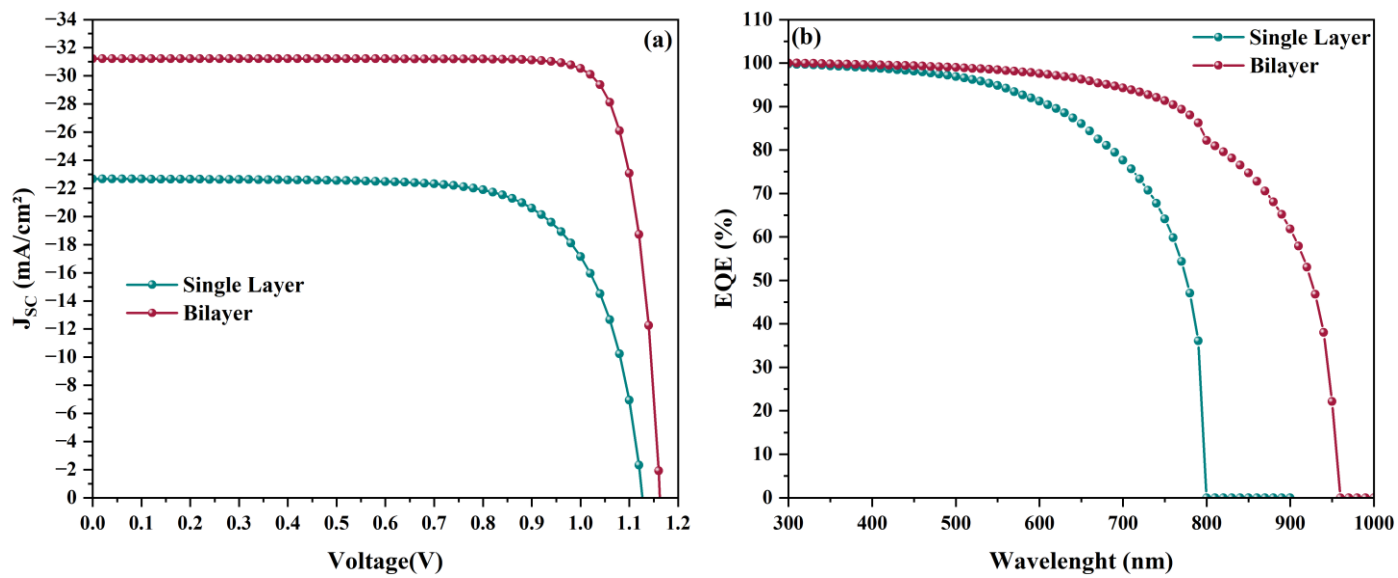


**Figure III.8:** Photovoltaic Performance Characterization (a) J-V characteristics and (b) External quantum efficiency spectra of Device I and Device II

**Table III.3** presents a comparison of the photovoltaic performance of different double-absorber solar-cell configurations based on theoretical (T) and experimental (E) studies. The reference Device-I, using MAPbI<sub>3</sub> as the absorber, exhibits a power conversion efficiency (PCE) of 18.55%, with a VOC of 1.12 V, a fill factor (FF) of 72.53%, and a JSC of 22.67 mA/cm<sup>2</sup>. In comparison, Device-III, employing a MASnI<sub>3</sub>/MAPbI<sub>3</sub> double-absorber configuration, shows a significant improvement, reaching a PCE of 30.15%. This enhancement is accompanied by higher VOC (1.17 V), FF (81.42%), and JSC (31.35 mA/cm<sup>2</sup>), demonstrating the beneficial effect of combining two absorber materials.

The results also show that the proposed Device-III configuration compares favorably with several previously reported theoretical and experimental double-absorber structures. For example, Sr<sub>3</sub>SbI<sub>3</sub> and Sr<sub>3</sub>PI<sub>3</sub> single-absorber configurations reported PCE values of 28.05% and

28.15%, respectively. Other double-absorber systems, such as MAPbI<sub>3</sub>/MASnBr<sub>3</sub> and CsPbI<sub>3</sub>/CsGeI<sub>3</sub>, achieved efficiencies of 25.91% and 24.06%, respectively. Experimental devices based on CsPbI<sub>3</sub>/Cs<sub>0.25</sub>FA<sub>0.75</sub>PbI<sub>3</sub> and CsPbI<sub>3</sub>/FAPbI<sub>3</sub> exhibited lower efficiencies of 17.39% and 15.60%, respectively, highlighting the generally higher performance predicted by theoretical studies.

Among the compared configurations, the Sr<sub>3</sub>SbI<sub>3</sub>/Sr<sub>3</sub>PI<sub>3</sub> double-absorber structure reported in Ref. [39] achieves the highest PCE of 34.13%, together with a VOC of 1.0981 V, FF of 87.29%, and JSC of 35.6145 mA/cm<sup>2</sup>. Although Device-III does not reach this maximum efficiency, its PCE of 30.15% remains competitive and is higher than most of the configurations listed in the table. In particular, its relatively high VOC, FF, and JSC indicate a favorable balance between voltage generation, charge collection, and overall device quality.

| Absorber Material                                                          | Type of works | V <sub>oc</sub> (V) | FF (%) | J <sub>sc</sub> (mA/cm <sup>2</sup> ) | PCE (%) | Ref.      |
|----------------------------------------------------------------------------|---------------|---------------------|--------|---------------------------------------|---------|-----------|
| Device-I (MAPbI <sub>3</sub> )                                             | T             | 1.12                | 72.53  | 22.67                                 | 18.55   | This work |
| Device-III (MASnI <sub>3</sub> / MAPbI <sub>3</sub> )                      | T             | 1.17                | 81.42  | 31.35                                 | 30.15   | This work |
| Sr <sub>3</sub> SbI <sub>3</sub>                                           | T             | 0.93                | 87.31  | 34.67                                 | 28.05   | [31]      |
| Sr <sub>3</sub> PI <sub>3</sub>                                            | T             | 0.92                | 87.55  | 34.65                                 | 28.15   | [32]      |
| CsPbI <sub>3</sub> /Cs <sub>0.25</sub> FA <sub>0.75</sub> PbI <sub>3</sub> | E             | 1.2                 | 76     | 18.91                                 | 17.39   | [33]      |
| CsPbI <sub>3</sub> /FAPbI <sub>3</sub>                                     | E             | 1.22                | 74     | 17.26                                 | 15.6    | [34]      |
| MAPbI <sub>3</sub> /MASnBr <sub>3</sub>                                    | T             | 1.04                | 78.18  | 31.77                                 | 25.91   | [35]      |
| CsPbI <sub>3</sub> /CsGeI <sub>3</sub>                                     | T             | 1.19                | 86.19  | 23.45                                 | 24.06   | [36]      |
| CsPbI <sub>3</sub> /FAPbI <sub>3</sub>                                     | T             | 1.1                 | 74     | 24.5                                  | 19.94   | [37]      |
| CsPbI <sub>3</sub> /CsSnI <sub>3</sub>                                     | T             | 0.96                | 78.41  | 26.59                                 | 19.99   | [38]      |
| Sr <sub>3</sub> SbI <sub>3</sub>                                           | T             | 1.0639              | 88.63  | 32.4022                               | 30.55   | [39]      |
| Sr <sub>3</sub> PI <sub>3</sub>                                            | T             | 1.0928              | 83.93  | 33.9365                               | 31.12   | [39]      |
| Sr <sub>3</sub> SbI <sub>3</sub> /Sr <sub>3</sub> PI <sub>3</sub>          | T             | 1.0981              | 87.29  | 35.6145                               | 34.13   | [39]      |

### III.11. Conclusions

This comprehensive numerical investigation of single-layer and bilayer perovskite solar cells reveals fundamental optimization principles for achieving high-efficiency photovoltaic devices. The systematic variation of device architecture, absorber thickness, shallow acceptor density, and defect trap density across extensive parameter spaces establishes several key findings.

The Device II bilayer configuration achieves a 55.4% absolute efficiency improvement compared with the single-layer Device I through extended spectral harvesting and optimized band alignment. Its maximum efficiency reaches 35.68% when optimal absorber thickness, doping concentration, and minimal defect density are simultaneously achieved. Variation of absorber thickness from 0.35 to 0.8  $\mu\text{m}$  increases PCE by 18.8%, from 26.55% to 31.54%. This improvement is primarily driven by an 11.2% enhancement in short-circuit current density ( $J_{\text{sc}}$ ), although it is partially offset by a 4.45 percentage-point degradation in fill factor (FF). Among the two absorber layers,  $\text{MASnI}_3$  thickness exerts approximately six times greater influence on device performance than  $\text{MAPbI}_3$  thickness.

Variation of shallow acceptor density produces a 23.7% improvement in PCE, increasing efficiency from 28.84% to 35.68%. This enhancement results from a synergistic improvement in FF of 9.6 percentage points and an increase in open-circuit voltage ( $V_{\text{oc}}$ ) of 0.119 V, despite a modest 1.6% reduction in  $J_{\text{sc}}$ . Furthermore, the presence of a broad robustness plateau covering approximately 30% of the investigated parameter space demonstrates that high performance can be maintained across a relatively wide range of doping concentrations. Defect trap density has the strongest influence on device efficiency, with its variation producing a 92.7% relative efficiency loss, from 30.53% to only 2.24%. This effect substantially exceeds the impacts associated with absorber thickness and doping, establishing defect reduction as the highest-priority optimization target. A critical threshold is identified at a trap density of ( $n_{\text{t}} < 10^{15} \text{ cm}^{-3}$ ), which is necessary to maintain efficiencies above 30%.

The results establish a clear optimization hierarchy in which material quality through defect reduction has the greatest impact, followed by electrical optimization through doping and then geometric optimization through absorber thickness. This hierarchy reflects the fundamentally different physical mechanisms involved, with defect-related losses exhibiting highly nonlinear or exponential behavior compared with the more gradual linear or logarithmic responses associated with geometric and electrical parameters.

The work function of the back contact significantly influences FF and  $V_{\text{oc}}$  while having a comparatively limited effect on  $J_{\text{sc}}$ . An optimal work function of 5.65 eV produces the maximum efficiency enhancement, with its beneficial effect being particularly pronounced in the bilayer architecture.

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## GENERAL CONCLUSION

This thesis has addressed the operation, modelling, and numerical optimization of perovskite solar cells, with emphasis on the relationship between device architecture, material parameters, carrier transport, recombination, and photovoltaic performance. The work was developed through three complementary parts: general principles of solar-cell operation, numerical simulation using SCAPS-1D, and a systematic optimization study of single-layer and bilayer perovskite devices. The overall approach reflects the current direction of perovskite photovoltaic research, in which high conversion efficiency must be accompanied by controlled defects, favorable interfaces, improved stability, and realistic device engineering [1,3,8-12].

### Overall Findings

The first part of the thesis established the fundamental concepts required to understand photovoltaic conversion and solar-cell performance. A photovoltaic device converts incident solar radiation into electrical power through photon absorption, generation of charge carriers, separation of electrons and holes, and selective extraction through the transport layers and electrodes. The analysis of photovoltaic parameters such as  $V_{oc}$ ,  $J_{sc}$ , FF, and PCE provides a common basis for evaluating the effect of material and architectural modifications. In the context of perovskite photovoltaics, the combination of strong absorption and tunable electronic properties explains the continuing interest in these materials, while their sensitivity to defects, interfaces, environmental conditions, and processing remains a major research challenge [3,7,10-11].

The second part established SCAPS-1D as the numerical framework for the device-level analysis. The simulator provides a physically consistent means of examining the electrostatic potential and carrier distributions through the coupled Poisson and continuity equations. The modelling framework makes it possible to vary individual material and interface parameters systematically and to identify how these parameters affect the resulting current-density-voltage characteristics. Recent studies confirm that SCAPS-1D remains a useful research tool for screening absorber materials, transport layers, defect densities, interface conditions, and device architectures before experimental fabrication [4-6].

## Single-Layer and Bilayer Device Optimization

The third part of the thesis investigated two device architectures: the single-layer FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/CuO/Au structure and the bilayer FTO/WS<sub>2</sub>/MAPbI<sub>3</sub>/MASnI<sub>3</sub>/CuO/Au structure. The results show that photovoltaic performance cannot be attributed to one parameter alone. Instead, it results from the combined effects of optical absorption, band alignment, carrier generation and transport, recombination, and carrier extraction. The comparison between the two architectures illustrates the potential of incorporating a narrower-band-gap absorber to extend spectral utilization beyond the range effectively exploited by a single MAPbI<sub>3</sub> absorber.

For the single-layer device, absorber thickness exhibited a non-monotonic influence on efficiency. Increasing the MAPbI<sub>3</sub> thickness enhanced light absorption and therefore increased  $J_{sc}$  over the investigated range, but excessive thickness was accompanied by a reduction in FF and a modest decrease in  $V_{oc}$ . The resulting optimum near the intermediate thickness demonstrates the classical trade-off between additional photon absorption and the electrical cost associated with longer carrier-transport paths. This observation is consistent with the broader device-engineering literature in which absorber thickness must be selected according to the balance between optical generation and charge collection rather than maximized independently.

The shallow acceptor-density analysis further demonstrated that electrical doping can strongly modify device behavior. An intermediate doping range provided improved FF and  $V_{oc}$ , whereas excessive doping resulted in pronounced performance deterioration. The physical interpretation is that moderate doping can strengthen the internal electric field and facilitate carrier extraction, while excessive dopant concentrations can increase recombination and disturb the favorable transport conditions required for efficient operation. The results therefore emphasize the importance of identifying a physically meaningful doping window rather than assuming that higher carrier concentration always produces better photovoltaic performance.

Defect-trap density produced the strongest degradation among the investigated parameters. Increasing the trap density introduced progressively stronger recombination losses, leading to simultaneous reductions in  $J_{sc}$ ,  $V_{oc}$ , FF, and ultimately PCE. In the bilayer simulations, the calculated efficiency decreased dramatically as the defect density increased,

while low defect densities preserved high photovoltaic performance. This finding is particularly important because recent experimental and review literature identifies bulk and interface defects, non-radiative recombination, and defect-induced instability as central barriers to further improvement of perovskite photovoltaics [1,3,8,11].

## **Importance of the Bilayer Architecture**

The bilayer architecture demonstrated the potential of combining absorbers with complementary band gaps. In the investigated MAPbI<sub>3</sub>/MASnI<sub>3</sub> configuration, the narrower-band-gap MASnI<sub>3</sub> layer provides access to longer-wavelength photons that are not efficiently converted by the wider-band-gap MAPbI<sub>3</sub> absorber alone. The numerical results consequently showed a substantial increase in J<sub>sc</sub> and overall PCE when the bilayer structure was optimized. The study also demonstrated that the thicknesses of the two absorbers do not necessarily have identical effects on device performance, reflecting their different roles in spectral absorption and carrier generation.

The simulated improvement of the bilayer device should, however, be interpreted as a numerical optimization result under the specified material parameters, interface properties, illumination conditions, and idealizations of the SCAPS-1D model. It should not be interpreted as a direct prediction of experimentally achievable efficiency without experimental validation. In particular, practical all-perovskite tandem devices must address phase stability, defect formation, interfacial recombination, chemical compatibility, processing complexity, and long-term operational stability. Recent reviews identify these factors as continuing limitations even as tandem efficiencies approach and exceed the performance of conventional single-junction technologies [1,8,9].

## **Main Scientific Conclusions**

- Perovskite solar-cell performance is governed by coupled optical, electrical, and interfacial processes; therefore, meaningful optimization requires simultaneous consideration of several device parameters.

- SCAPS-1D provides a practical numerical framework for evaluating the effects of absorber properties, transport layers, defect states, interfaces, and contact conditions on photovoltaic performance.
- Absorber thickness must balance photon absorption against carrier-transport and recombination losses; increasing thickness does not necessarily lead to monotonic improvement in PCE.
- Moderate shallow acceptor concentrations can improve carrier extraction and voltage generation, whereas excessive doping can introduce detrimental recombination and transport effects.
- Defect-trap density is a particularly influential parameter because trap-assisted recombination can strongly reduce photocurrent, voltage, fill factor, and overall efficiency.
- Combining wide- and narrow-band-gap perovskite absorbers provides a numerical route to broader spectral utilization and higher current generation than the corresponding single-absorber configuration.
- The performance of an optimized numerical device remains conditional on the assumed material parameters and interface properties; experimental fabrication, characterization, and stability testing are required to validate the predicted performance.
- Future development should therefore combine device-level modelling with experimental defect characterization, interface engineering, stability testing, scalable processing, and environmental assessment.

## Perspectives and Future Work

The results provide several directions for future research. First, the numerical parameter set can be extended to include temperature-dependent material properties, series and shunt resistances, wavelength-dependent optical generation, and more detailed bulk and interface recombination models. Second, the simulated architectures should be subjected to experimental validation through fabrication and characterization of the individual transport layers, absorber films, and complete devices. Third, particular attention should be paid to the stability of the narrow-band-gap absorber and to interfacial losses in the bilayer configuration. These issues are especially important because recent tandem research identifies wide-band-gap stability,

interfacial recombination, and scalable processing as key barriers to practical deployment [1,8,9].

Further studies could also integrate first-principles calculations with device simulation. Density-functional-theory calculations can provide band structures, band gaps, dielectric properties, effective masses, defect energetics, and other material descriptors, while SCAPS-1D can translate selected material parameters into device-level predictions. Such a multiscale strategy would reduce the dependence on assumed parameters and could provide a more physically grounded pathway for designing new absorber and transport-layer combinations. This direction is consistent with recent studies that combine first-principles calculations with SCAPS-1D for perovskite-device design [5].

Finally, the development of perovskite photovoltaics should be assessed using a broader set of criteria than peak PCE alone. Operational lifetime, reproducibility, large-area performance, lead management, environmental impact, material availability, and manufacturing cost are increasingly important for evaluating technological maturity [10-12]. The numerical results obtained in this thesis therefore represent one component of a wider research strategy: numerical optimization can identify promising device configurations and physical trends, while experimental validation and stability assessment determine whether these configurations can be translated into reliable photovoltaic technologies.

In conclusion, the thesis demonstrates that systematic numerical modelling can provide valuable insight into the optimization of perovskite solar-cell devices. The comparison between single-layer and bilayer architectures shows the potential of band-gap engineering for improving spectral utilization, while the parameter analysis emphasizes that defect control, appropriate electrical properties, and suitable absorber thickness are all essential for achieving high performance. The work consequently provides a foundation for further experimental and computational studies aimed at developing efficient, stable, and scalable perovskite photovoltaic devices.

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## الملخص

يقدم هذا العمل دراسة عددية للخلايا الشمسية القائمة على مواد البيروفسكايت باستخدام برنامج SCAPS-1D ، مع التركيز على تأثير بنية الطبقة الماصة على أداء الجهاز. تمت دراسة بنيتين: بنية ذات طبقة ماصة واحدة قائمة على  $\text{MAPbI}_3$  ، وبنية ذات طبقتين ماصتين من  $\text{MAPbI}_3/\text{MASnI}_3$  ، ضمن تراكيب من نوع  $\text{FTO}/\text{WS}_2/\text{absorber}/\text{CuO}/\text{Au}$ . تم تحليل تأثير سمك الطبقة الماصة، وتركيز الشوائب القابلة، وكثافة العيوب، ودالة الشغل للقطب الخلفي بشكل منهجي على المعلمات الكهروضوئية. كما أُجريت مقارنة بين البنيتين من حيث نقل حوامل الشحنة، وجمع الشحنات، وكفاءة تحويل الطاقة الضوئية. وتوفر النتائج فهماً أفضل للعوامل الفيزيائية المتحكم في أداء الجهاز، وتساعد على تحديد الشروط المناسبة لتحسين أداء الخلايا الشمسية القائمة على البيروفسكايت ذات البنية ثنائية الطبقة.

## Abstract

This work presents a numerical study of perovskite solar cells based on SCAPS-1D, focusing on the effect of absorber architecture on device performance. Single-layer  $\text{MAPbI}_3$  and bilayer  $\text{MAPbI}_3/\text{MASnI}_3$  configurations are investigated using  $\text{FTO}/\text{WS}_2/\text{absorber}/\text{CuO}/\text{Au}$  structures. The influence of absorber thickness, acceptor concentration, defect density, and back-contact work function on the photovoltaic parameters is systematically analyzed. A comparative assessment of the single-layer and bilayer configurations is performed in terms of carrier transport, charge collection, and power conversion efficiency. The results provide a physical understanding of the parameters governing device performance and identify suitable conditions for the optimization of bilayer perovskite solar cells.

## Résumé

Ce travail présente une étude numérique de cellules solaires à base de pérovskites à l'aide du logiciel SCAPS-1D, portant sur l'influence de l'architecture de l'absorbeur sur les performances du dispositif. Deux configurations sont étudiées : une structure à couche absorbante unique à base de  $\text{MAPbI}_3$  et une structure à double couche  $\text{MAPbI}_3/\text{MASnI}_3$ , intégrées dans des architectures  $\text{FTO}/\text{WS}_2/\text{absorbeur}/\text{CuO}/\text{Au}$ . L'influence de l'épaisseur de l'absorbeur, de la concentration en accepteurs, de la densité des défauts et du travail de sortie du contact arrière sur les paramètres photovoltaïques est systématiquement analysée. Une comparaison des deux configurations est réalisée en termes de transport des porteurs, de collecte des charges et de rendement de conversion photovoltaïque. Les résultats permettent de mieux comprendre les paramètres physiques régissant les performances du dispositif et d'identifier des conditions appropriées pour l'optimisation des cellules solaires à pérovskite à double couche.