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Computational study of $CuAlO_2$/ZnO, and NiO/ZnO Perovskite Solar Cells by Numerical Simulation

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ABSTRACT

This study presents a comparative analysis of the performance of $CuAlO_2$/ZnO and NiO/ZnO perovskite solar cells employs numerical simulation with an emphasis on temperature flactuations, layer thicknesses and electrical propeties using the SCAPS-1D modlling tool, the photovoltaic parameters such as open circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF), and power convrsion efficiency (PCE) were invstigated under standard test conditions and varying operational senarios. The effects of the hole transport layer (HTL) materials ($CuAlO_2$ and NiO) on device performace were assessed with particular attention to their band alighment, carrier mobility, and defect density. Results indicate that $CuAlO_2$ structure achieves higher efficiency due to better band alghment and charge transport properties compared to NiO/ZnO. However, the NiO-based device demostrated superior thermal stability over a wide temperature range. Optimization of HTL thickness and defect density further enhaned device performance with $CuAlO_2$ exhibiting optimal peformance at lower defects densities. This comparative study provides an insights into material selection an design parameters for efficient and stable perovskite solar cells

Keywords: Perovskite solar cell, $CuAlO_2$/ZnO, NiO/ZnO, SCAPS-1D, PCE, HTL, ETL, Voc, Jsc

INTRODUCTION

Global demand for the renewable energy has driven extensive research in to the developmentof high-efficiency and cost-effective solar cells. Among various photovoltaic technologies, perovskite solar cells (PSCs) have generated considersble attention as a result of their impressive power conversion efficiencies (PCE), scalability, and relatively low production costs (Danladi *et al.,*2021). Over the past decade aluminium oxide and zinc oxide have emerged as potential canditates for improving the electron and hole transport layers in PSCs, offering favourable electrical and optical properties . This study investigates the perfomance enhancement of $CuAlO_2$/ZnO and NiO/ZnO-based perovskite solar cells through numerical simulation, with a view to achieving enhanced efficiency. The numerical approach enables a detailed analysis of device parameters, including band alligment, charge carrier dynamics and recombination mechanism, allowing for optimized design and material selection. The results of this simulation using solar capacitance simulator (SCAPS-ID) is expected to provide valuable insights into the potential of $CuAlO_2$/ZnO and NiO/ZnOstructures for next generation perovskite solar cells contributing to the ongoimg effort to improve the effiency and viability of PSC technology.The use of Perovskite solar cells has gained intrest due to their exceptional effectiveness, tunable band gap and low manufacturing costs. The key to performance improvement lies in optimizing both the perovskite absorber layer and the tranport layers, which facilitate charge exrtraction and reducerecombination loses

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(Hossain *et al*.,2022).Perovskite is a type of mineral that was found in the Ural Mountains and named after Lev Perovskite (the founder of Russian geographical society); true perovskite is composed of Calcium, Titanium and Oxygen in the form $CaTiO_3$ with a structure of thE form ABX3. A Perovskite compound are of the same form with the same Crystallography as the Perovskite mineral (Tala-Ighil Zaïr1, 2021). The crystal structure of the form ABX3 is represented in Figure1 below:

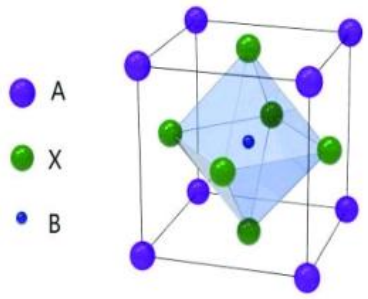

Figure 1: ABX3 perovskite cystal structure.

The first perovskite applied to solar cells was used in 2012. The materials ABX3 is composed of: A = an organic Cation - methylammonium (CH3NH3+) or Formamidinium (NH2CHNH2+). B = an inorganic Cation - usually lead (II) (Pb2+). X3= A Halogen Anion – usually Chloride (Cl-) or Iodide (I-) (Tala-Ighil Zaïr, 2021).Perovskite solar cells have rapidly gained attention due to their high power conversion efficiencies, which have reached over 25% in laboratory conditions, approaching the efficiency of traditional silicon-based solar cells. The materials used for perovskite solar cells can be processed using low-cost methods, such as solution processing, which allows for cheaper and scalable manufacturing compared to silicon solar cells. The solar cells can be made on flexible substrates, which opens up possibilities for applications in various settings, such as portable electronics and building-integrated photovoltaics. The composition of perovskite materials can be changed to modify their bandgap which enables tuning of the absorption spectrum for different light conditions. They can be fabricated using simpler and more cost-effective techniques, such as spin-coating, inkjet printing, or vapor deposition, reducing manufacturing complexity and cost (Suresh and Chandra 2021).

The objectives of the work are

i. To Examine how varying the thickness of the $CuAlO_2$/ZnO and NiO/ZnO layers influences the overall efficiency and performance of the solar cells.

ii. To evaluate the temperature dependence, thermal stability and efficiency of the CuAlO2/ZnO and NiO/ZnO perovskite solar cells across a range of operating temperatures

iii. To Identify which configuration (CuAlO2/ZnO vs. NiO/ZnO) provides superior photovoltaic performance and why

Perovskite solar cells (PSCs) have revolutionized the field of photovoltaic research since their inception, thanks to their exceptional power conversion efficiency (PCE) and cost-effective manufacturing processes. (Amu, 2014) The perovskite material, typically a hybrid organic-inorganic lead halide, serves as the light-harvesting layer, exhibiting a high absorption adjustable bandgap and outstanding charge carrier mobility. Despite these advantages, the extended stability of PSCs remains a major obstacle, particularly under environmental stresses such as humidity, temperature fluctuations, and UV exposure (Dong *et al*,. 2015) One of the crucial components in PSCs that affects both efficiency and stability is the hole-transport material (HTM). HTMs are

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responsible for extracting holes from the perovskite layer and moving them to the anode (Eli, *et al* 2019) Traditionally, organic HTMs, especially Spiro-OMeTAD, have been widely used due to their high PCEs. However, these materials often suffer from high cost, complex synthesis, and stability issues, which has led to increased interest in inorganic alternatives (Green *et al* 2014).

According to Yang *et al.,* 2018. Perovskite solar cells (PSCs) based on organic-inorganic hybrid lead trihalide perovskites have recently exhibited great potential of producing low cost solar electricity the power conversion efficiency (PCE) of PSC has been skyrocketed from the initial 3.8% in 2009 to current 22.7% within 7years. While organic HTMs like Spiro-OMeTAD have historically been the standard, their drawbacks have prompted researchers to explore inorganic materials as potential alternatives. Inorganic HTMs, such as $CuAlO_2$, NiO, and ZnO have attracted attention due to their inherent advantages over organic counterparts. These include superior thermal stability, chemical robustness, and lower production costs. However, the application of these materials in PSCs is still relatively underexplored, and their performance as HTMs needs to be thoroughly investigated (Lingyan *et al.,*2019). Copper aluminum oxide ($CuAlO_2$) is a p-type semiconductor with a Delafossite structure, known for its wide bandgap (~3.5 eV), high thermal stability, and good electrical conductivity. Several studies have explored the potential of $CuAlO_2$ in various electronic applications, but its use as an HTM in PSCs is still emerging (Lingyan, *et al*., 2019). $CuAlO_2$ has been synthesized using various methods, including solid-state reactions, sol-gel processes, and hydrothermal techniques. Its p-type conductivity arises from copper vacancies or oxygen interstitials (Takashi and Takoyashi 2016).

The material's wide bandgap and suitable energy level alignment with the perovskite absorber layer make it a promising candidate for HTM applications. Early researches have demonstrated CuAlO's potential as a transparent p-type conductor in optoelectronic devices, but studies on its application in PSCs are limited (Mohammad *et al.,* 2020) $CuAlO_2$ is a very promising delafossite material for optoelectronic uses for several reasons. For instance, it shows better optical transparency in the visible range than $CuCrO_2$ while also keeping in strong electrical conductivity, (Achilease *et al*.,2019). However, more research is needed to optimize its performance and fully understand its interaction with the perovskite layer. Zinc oxide (ZnO) is a versatile material widely used as an electron transport material (ETM) in PSCs due to its wide bandgap (~3.37 eV), high electron mobility, and chemical stability (Ajay *et al.,* 2012). However, recent studies have explored its potential as a dual-function material, serving both as an ETM and HTM.ZnO's versatility comes from its ability to be doped with various elements to adjust its electronic properties. By doping ZnO with elements such as Al, Ga, or Li, researchers can shift its energy levels to make it more suitable as an HTM (Bett *et al.,* 2024). The main challenge with using ZnO as an HTM is its inherent n-type conductivity, which must be carefully controlled through doping to ensure efficient hole transport. Studies have shown that while ZnO can be engineered to function as an HTM, its performance is still inferior to traditional HTMs, and further optimization is required. Research into ZnO as an HTM is still in its early stages.

Initial results indicate that with appropriate doping and interface engineering, ZnO can serve as a viable HTM in PSCs. However, its dual functionality remains a subject of ongoing investigation (Lin *et al.,* 2017).

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Indium tin oxide (ITO) is one of the most widely used transparent conducting oxides (TCOs) in the electronics industry due to its high electrical conductivity and optical transparency (Yu *et al.,* 2016) While ITO is traditionally used as an electrode in PSCs, its potential as an HTM is underexplored.ITO has a high work function (typically ~4.7 eV), which can align well with the valence band of the perovskite layer, facilitating hole transport (Pradeepkumar *et al.,* 2015) Its excellent conductivity and transparency make it an attractive candidate for HTM applications in PSCs. Most research on ITO has focused on its use as an electrode rather than an HTM. However, a few studies have investigated its potential as an HTM, showing that with proper interface engineering, ITO could function as an effective HTM. The challenge lies in balancing its dual role as both a conductor and a hole transporter, which requires careful material and interface optimization (Hui-Jing *et al*., 2017).

The Solar Cell Capacitance Simulator (SCAPS-1D) is a widely-used tool for simulating the performance of solar cells, including PSCs. SCAPS-1D allows researchers to model the physical and electronic properties of various layers within a solar cell, providing insights into the behavior of different materials and interfaces.SCAPS-1D has been used extensively to model the performance of PSCs, allowing researchers to simulate different HTMs, ETMs, and absorber materials (Jayan and Sebastian, 2021). The software enables the study of energy level alignment, charge transport dynamics, and recombination losses, providing a powerful tool for optimizing solar cell performance.. Numerous studies have used SCAPS-1D to simulate the performance of various HTMs in PSCs, helping to identify promising materials and guide experimental work. For instance, simulations have been used to optimize the thickness of HTM layers, study the impact of doping, and evaluate the stability of different material combinations under various environmental conditions (Minbashi *et al*., 2018) The study of $CuAlO_2$, ZnO, and NiO as HTMs in PSCs presents a promising avenue for improving the efficiency, stability, and cost-effectiveness of these devices. (Femi *et al.,* 2015) By leveraging the capabilities of SCAPS-1D, researchers can gain a deeper understanding of these materials' potential and guide the development of next-generation PSCs. This literature review highlights the importance of continuing research in this area, with a focus on optimizing inorganic HTMs and integrating them into stable, high-performance PSCs.

Enhancement of the $CuAlO_2$/ZnO and NiO/ZnO Perovskite Solar Cells

Efficiency Improvement: The total power conversion efficiency (PCE) of a $CuAlO_2$/ZnO and NiO/ZnO perovskite solar cell can be predicted through simulations by considering factors such as the open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and series and shunt resistances. Numerical simulations allow for adjusting these parameters to improve the effectiveness of power conversions. To simulate the performance enhancement of a $CuAlO_2$-ZnO and NiO/ZnO Perovskite solar cell numerically, the key theoretical background needs to be understood and involves various physical processes such as charge transport, light absorption, recombination processes, and the overall device architecture. The primary aim is to create a model and simulate how performance improves based on certain factors, such as open circuit voltage (Voc) fill factor (FF), conversion and quantum efficiencies, (1)–(6).

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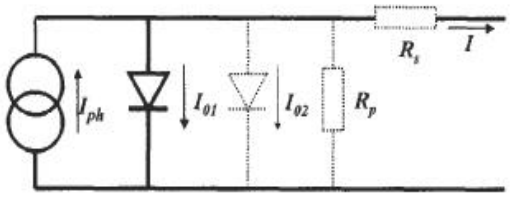

Figure 2: Equivalent circuit of a solar cell.

$$V_{oc} = \frac{kT}{q} ln\left(1 + \frac{I_{ph}}{I_o}\right) \text{.....} (1)$$

where

I_{ph} is the light generated current, I_o is the ideal diode current.

$$J_{sc} = \frac{I_{sc}}{A} \text{----------} (2)$$

where,

J_{sc} is the current density, I_{sc} is the short circuit current, and A is the surface area of the cell.

$$FF = \frac{P_{max}}{V_{oc}I_{sc}} = \frac{V_m I_m}{V_{oc}I_{sc}} \text{----------} (3)$$

FF is the fill factor, P_{max} is the maximum power output.

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_m I_m}{P_{in}} \text{----------} (4)$$

where

$\eta$is the conversion efficiency, Pin is the maximum power input, V_m is the maximum voltage, and I_m is the maximum current.

The solar cell parameters can just be deduced from the I-V characteristics curve as seen in Figure 3.The energy band gap can be determined using Eq. (5).

$$\alpha hv = A\left(hv - E_g\right)^n \text{.....} (5)$$

where,

A is a constant, E_g is the energy band gap and n determine the transition between valence band and conduction band, n is equal to 0.5 and 2 for indirect and direct transitions, respectively.

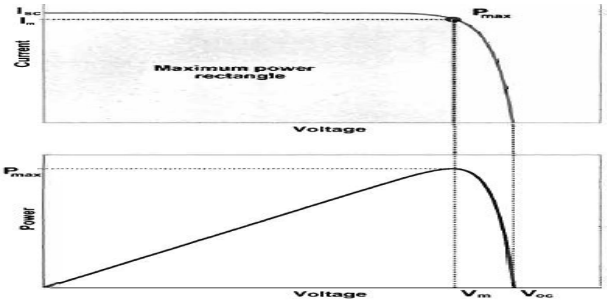

Figure 3: I-V characteristics of a solar cell.

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The quantum efficiency η_q is define as;

$$\eta_q = (1-R)\ \xi\ \left[1-\exp(-\alpha d)\right] \quad \text{.....(6)}$$

Where,

R is the reflectivity of the surface, ζ is the fraction of generated electron-hole pairs that contribute to the current, d is the thickness, and α is the absorption coefficient

The absorption process can be described by the Beer-Lambert law, which relates the light

intensity to the absorption coefficient:

$I(x) = I_0 e^{-\alpha(x)x}$---------- (7)

Where,
$I(x)$ is the light intensity at position x within the material.
I_0 is the incident light intensity at the surface.
$\alpha(x)$ is the absorption coefficient at position x, which depends on the material and the

Wavelength of light,
The generation rate of electron-hole pairs per unit volume is given by:

$G(x) = \alpha(x)\,.\,I_o e^{-\alpha(x)x}$---------- (8)
The movement of charge carriers (electrons and holes) in solar cell is usually controlled

by the drift-diffusion equations, these equations consider how carriers move because of an electric field.

The transport equations for electrons and holes are:

For electrons
$\frac{\partial n}{\partial t} = D_n \nabla^2 \mathrm{n} - \mu_\mathrm{n} \mathrm{E}\,.\,\nabla_\mathrm{n} + \mathrm{G_n}$ ----------(9) :
For holes

$\frac{\partial p}{\partial t} = D_p \nabla^2 \mathrm{p} - \mu_\mathrm{p} \mathrm{E}\,.\,\nabla_\mathrm{n} + \mathrm{G_p}$ ----------(10):
Where:
n and p are the electron and hole concentrations.
$D_n$and D_p are the diffusion coefficients for electrons and holes.

$\mu_\mathrm{n}$and $\mu_\mathrm{p}$are the mobility of electrons and holes.
$E$is the electric field.
$\mathrm{G_n}$and$\mathrm{G_P}$ are the generation rates of electrons and holes (from the absorption process)
(Mohammed, *et al.,*2020)

In a solar cell, the generated electron-hole pairs can recombine before they contribute to the photocurrent. The recombination rate (both radiative and non-radiative) is critical in determining the efficiency of the device. A common approximation for the total recombination rate is given by:

$R_{tot} = A\,.\,(n\,.\,p - n_{eq}.P_{eq})$---------- (11)

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Where:
$A$is the recombination constant.
n_{eq} and P_{eq} are the equilibrium carrier densities.
$n$and p are the electron and hole densities.

There are also specific models for Shockley-Read-Hall (SRH) recombination and Auger recombination, which can be included depending on the material properties.

The current density-voltage (J-V) characteristic of the solar cell is key for evaluating performance. The current density is given by the sum of the drift and diffusion currents:

$J = q\,.(\mu_n nE + D_n\nabla n + \mu_p pE + D_P)$---------- (12)

Where:
q is the charge of the electron.
n and p are the electron and hole densities.

μ_n , μ_p , D_n , D_P and are the mobilities and diffusion coefficients.

Simulating the Performance

To simulate the performance enhancement of the $CuAlO_2$-ZnO and NiO/ZnO perovskite solar cell, the following system of equations for current density, voltage, and carrier densities: will be investigated

Poisson equation for the electrostatic potential in the device:

$\nabla^{n}\varphi = \frac{q}{\epsilon}(n - P + N_d - N_a)$---------- (13)

Where,
φ is the electrostatic potential.
$N_d and N_a$and are the donor and acceptor densities.
$\in$is the permittivity of the material.

To numerically simulate the performance enhancement of the $CuAlO_2$-ZnO and NiO-ZnO Perovskite solar cells, a combination of equations describing light absorption, charge carrier transport, recombination, and current-voltage characteristics must be solved. These equations typically require numerical methods such as finite element analysis to solve, and performance can be optimized by adjusting material properties, layer thicknesses, and device architecture.

MATERIALS AND METHODS

The materials and methods employed in the numerical simulation study to enhance the perfomance of $CuAlO_2$/ZnO and NiO/ZnO based perovskite solar cells is a SCAPS ID simulation tool. The approach involves modelling and simulation to predict the behaviour of the solar cellS structure and optimize its performance through parameter adjustments.

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Table 1: Materials Parameter Input.

Parameter	$CuAlO_2$	NiO	Perovskite	ZnO
Thickness (nm)	90	80	320	80
Bandgap Eg (eV)	3.46	3.700	1.600	3.200
Electron affinity, χ (eV)	2.5	2.100	4.100	4.100
Relative permitivityε_r	60	10.700	10.000	8.100
Conduction band effective densityof statesNc NC (cm^3)	1.00E16	2.000E+19	2.000E+18	4.500E+18
Balance band effective density of states N_v (cm^3)	1.00E18	1.000E+19	1.000E+18	1.000E+18
Electron mobility μ_e (cm^2/(V s))	2	1.2000E+1	1.000E+2	3.000E+2
Hole mobilityμ_p (cm^2/(V s))	8,6	2.000E+0	1.000E+1	1.000E+0
Donor density ND (cm^3)	0	0	1.000E+9	1.000E+19
Acceptor density NA (cm^3)	3.6 x18	1.6000E+14	1.000E+9	0
Electron thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
Hole thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7

Simulation of Perovskite Solar Cell

Figure 4 and 6 show the structure of the PSCs, in which Figure 4 consisted of front contact (ITO,) an ETL (ZnO), absorber layer (perovskite), a HTL ($CuAlO_2$), and a back contact (Ag), while Figure 5 consisted of front contact (ITO) an ETL (ZnO), perovskite. The absorber, a HTL (NiO), and a back contact (Ag) formed the basic structures for simulating PSCs. We used SCAPS 1D to carry out the simulation. In a photoelectric cell, sunlight photons hit the cell, creating electrons that are collected at the front contact via the ETL. The holes created by this process are gathered at the back contact through the HTL. This entire operation produces an electric current. By collecting electrons at the front and holes at the back contacts, we create a potential difference across the device. This potential difference is what generates electrical current in the device. All simulations were conducted at 300 K with an illumination of 100 mW/cm² and using an AM 1.5 G light spectrum. Table 1 displays the parameters for the simulation, including those from earlier research (Farhana, 2023). We also considered neutral-type defects with a single energetic distribution located in the middle of the bandgap for each material.

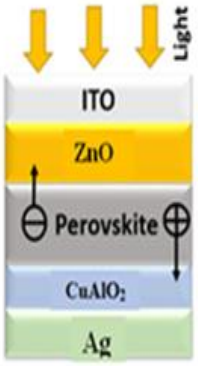

Figure 4: ITO, ZnO, Perovskite, $CuAlO_2$, Agdevice structure.

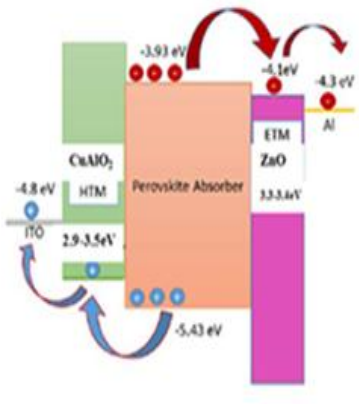

Figure 5: Schematic of device energy level.

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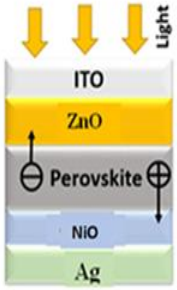

Figure 6: ITO, ZnO, Perovskite, $CuAlO_2$, Ag device structure.

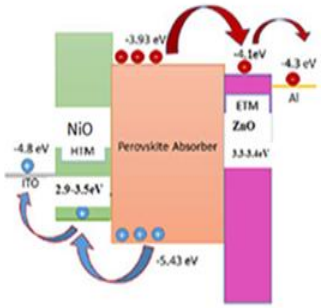

Figure 7: Schematic of device energy lev

Material Parameter Input

Front Contact ITO thickness 0.1µm ZnO (Zinc Oxide) An electron transport layer (ETL) thickness range ~0.02-0.050µm Perovskite Layer efficiently absorbs light and generates exitons that dissociates into free electrons thickness ~0.300-0.600nm $CuAlO_2$ (Copper Aluminium Oxide) A hole transport layer (HTL) thickness ~0.020-0.040nm NiO (Nickel Oxide) A hole transport layer (HTL) thuickness ~0.020-0.040nm Back contact: Silver (Ag) deposited to serve as back contact thin layer layer ~0.1µm to extract and conduct electrons to the external circuit and maintain low resistance for efficient current flow. Band gaps $CuAlO_2$ (~ 3.5-3.9eV), NiO(~ 3.5-4 eV) ZnO (~3.3 eV) Perovskite (~1.5-1.6 eV) Device Setup: Layer thickness optimization ($CuAlO_2$, NiO, ZnO, and perovskite) Adjustment for the interface between the layers to model charge transfer processes considering the work function and potential barrier.

Scaps 1D Simulation Software

The SCAPS-1D software, version 3.3.10 fig 8 was designed by the Department of Electronics and Information Systems (ELIS) at the University of Gent, Belgium (Pauwels and Vahoutte 2007), will be used to simulate the DC and AC electrical characteristics of the thin film heterojunction. This software can numerically fabricate solar cells by adding up to seven layers and is based on semiconducting equations such as Poisson's and continuity equations (Marlein and Burgelman 2007). The default Left and Right contacts were used, and optoelectrical parameters of every heterojunction layer were input parameters for the simulation. The software provides results and graphs for open circuit voltage (Voc), short circuit current density (Jsc), fill factor (FF), and quantum efficiency (QE%) which is similar with the work of (Marlein and Burgelman 2007).

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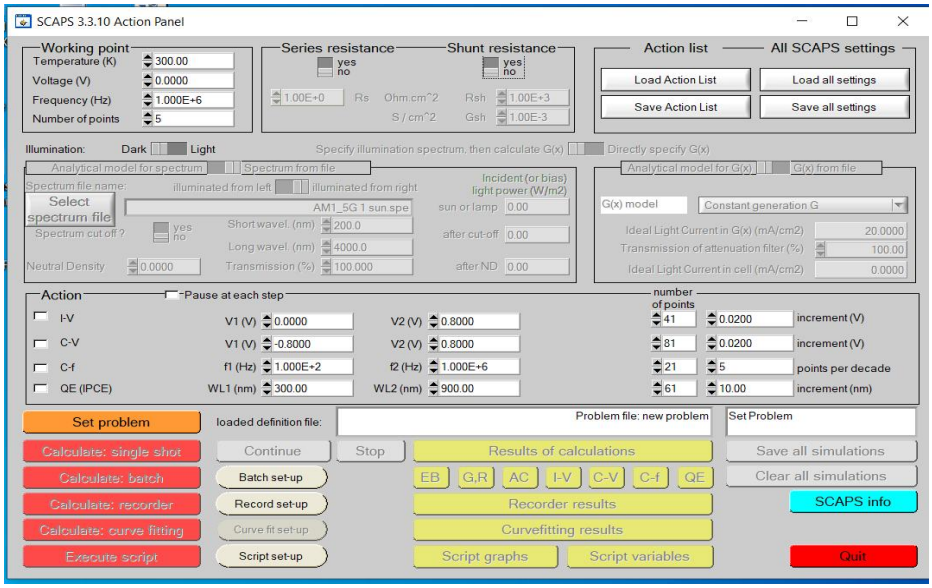

Figure 8: SCAPS 1D 3.3.10.

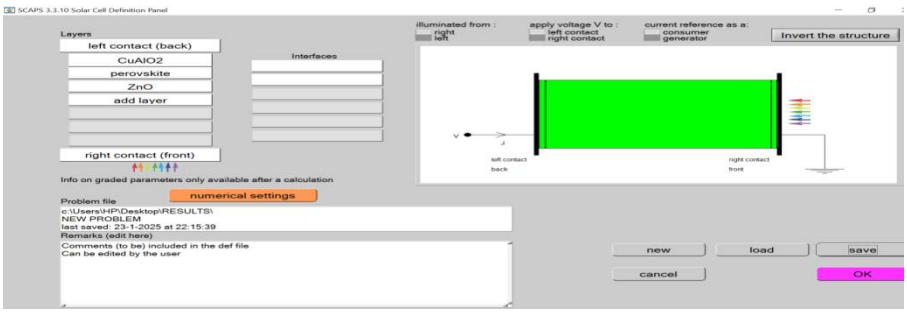

Figure 9: Simulated $CuAl_2$/ZnO perovskite solar cell.

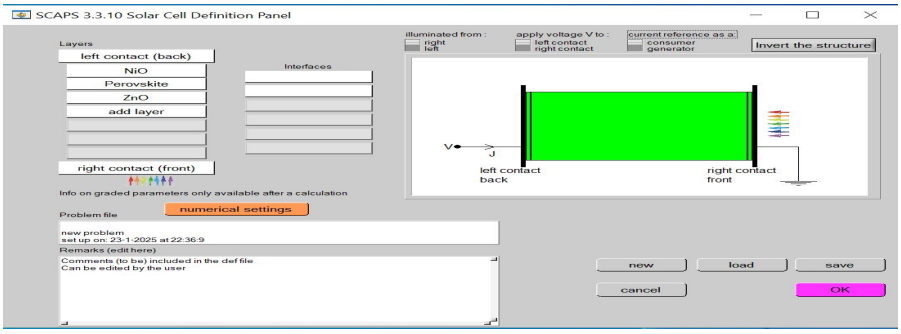

Figure 10: Simulated NiO_2/ZnO perovskite solar cell.

Illumination source AM1.5G spectrum with an intensity of 1000w/m^2 used to simulate standard sunlight, External vias voltage sweep (from 0V to open circuit voltage Voc) Variation of temperature (300 to 400K), in eleven steps, Series and shunt resistances incorperated to model practical loses Here each of the three layers of the perovskite solar cells 1- $CuAlO_2$, perovskite, ZnO and 2-NiO perovskite ZnO were taken separately and the solar cells simulated. The SCAPS programs compute energy bands, concentrations, currents, J-V characteristics, AC characteristics and spectral response at a specific working point (also with bias light or voltage) similar to the work of (Zioloa, 2016).

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The left and right contact were given, and light is applied from right contact and voltage is given to left contact and right contact is grounded. Interfaces were also added. First the structure is simulated, and J-V characteristics and C-V characteristics were noted. The SCAP software's numerical portion is depicted in figure 8.

The thin-film planar $CuAlO_2$/perovskite//ZnO and NiO/perovskite//ZnO heterojunction solar cell structures that were built and employed in the SCAPS simulations were shown in figure 9 and 10. The analysis was performed on the effects of the temperature, layer thicknesses and electrical properties of the perovskite layer.The performance of the $CuAlO_2$/perovskite/ZnO and NiO/perovskite/ZnO planar heterojunction thin-film solar cell under various solar concentrations and operating temperatures were also examined. Table 1 lists the parameters for $CuAlO_2$ NiO, perovskite, and ZnO that were used in the simulations.

RESULTS AND DISCUSSIONS

Variation in Temperature

Temperature significantly affects the efficiency of heterojunction solar cells. Figures 12 and 14 revealed that following trends: Open Circuit Voltage (Voc) Both $CuAlO_2$/ZnO and NiO/ZnO cells experience a decline in Voc as temperature increases. This happens due to an increase in carrier recombination and a reduction in bandgap energy. NiO/ZnO might show better thermal stability due to NiO's higher tolerance to temperature-induced degradation. The open circuit voltage (Voc) of a solar cell generally decreases as the temperature increases from 300K-400K.this can still be observed in figures 12 and 14 for $CuAlO_2$/ZnO and NiO/ZnO perovskite solar cells this is due to the shrinking behavior of a semiconductor with increase in temperature and leads to a lower built-in potential and consequently a lower open circuit voltage (Voc), also the reverse saturation current Voc as calculated approximately using equ.1 increases exponentially with increase in temperature which leads to a reduction in Voc Here NiO/ZnO typically shows a higher saturation current Jo than CuAlO2/ZnO and the temperature dependence is stronger due to higher carrier activation and recombination. For open circuit voltage $CuAlO_2$/ZnO typically has a higher Voc than NiO/ZnO, and the Voc drop with temperature is more significant in NiO/ZnO due to its higher recombination rate, this result is in agreement with the findings of (Priyanka *et al*., 2020).

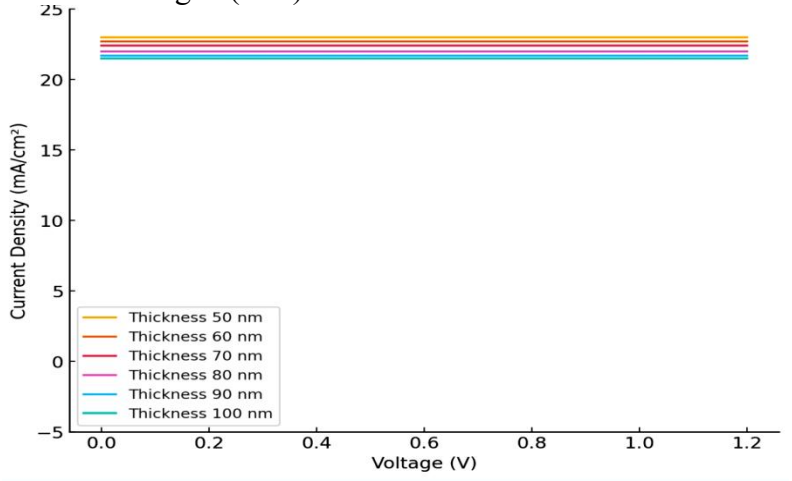

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Figure 12 I-V characteristics of $CuAlO_2$/ZnO perovskite solar cells

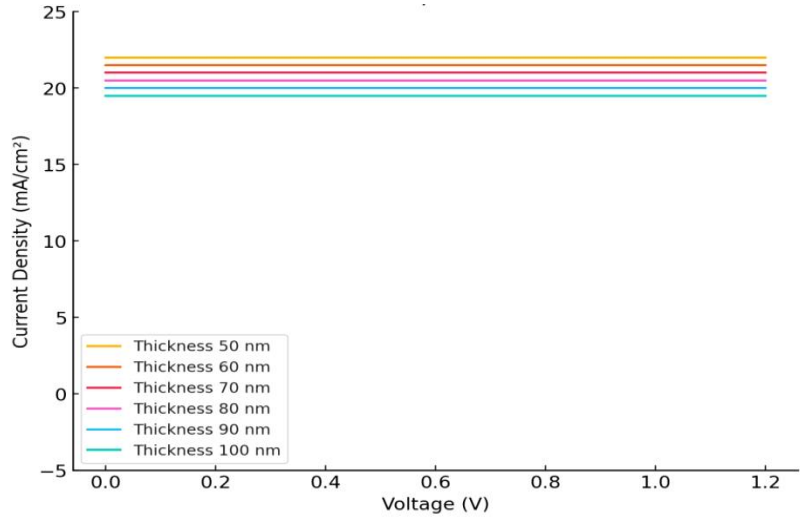

Figure 13: I-V characteristics for NiO/ ZnO perovskite solar cell.

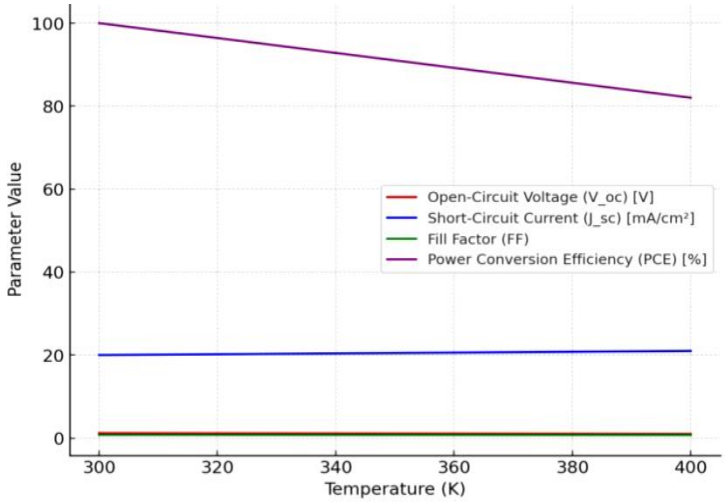

Figure 14: effect of temperature on $CuAlO_2$/ZnO perovskite solar cell.

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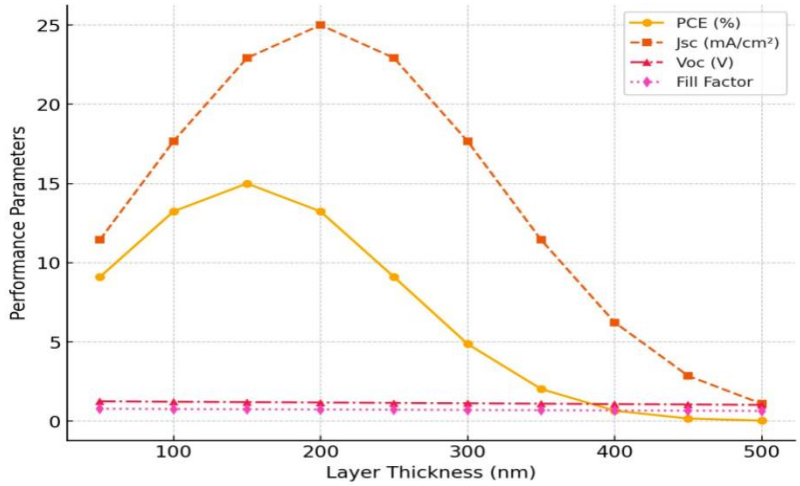

Figure 15: effect of layer thickness on $CuAlO_2$/ZnO perovskite solar cell.

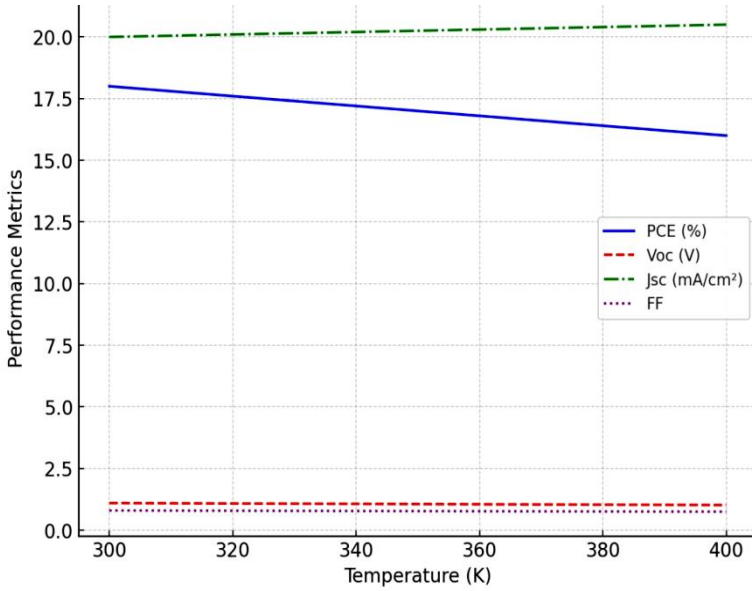

Figure 16: Effect of Temperature on NiO/ZnO perovskite solar cell.

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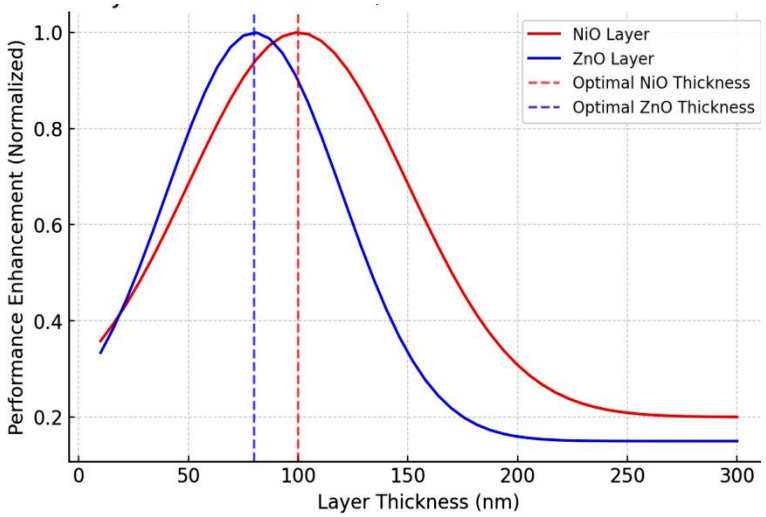

Figure 17: Effect of layer thickness on NiO/ZnO perovskite solar cell.

Variation in Layer Thickness

Optimizing the thicknesses of $CuAlO_2$/ZnO and NiO/NiO layers significantly influences the performance of perovskite solar cells. Maintaining an optimal balance (~50-100nm) for both HTL and ETL ensures better charge extraction, lower recombination losses, and improved PCE (Ahmed *et al.,*2018). Figures 13 and 15 shows the graphs of the variations of layer thicknesses for HTLs ($CuAlO_2$ and NiO) and ETL (ZnO) it could be observed that in both heterojunctions both rely on careful optimization of layer thicknesses for effective charge transport. $CuAlO_2$ has a better transparency but higher resistivity compared to NiO requiring a thinner layer for optimal performance, while NiO based structure tend provide better stability and energy level matching with perovskite though excessive thickness reduces efficiency and ZnO excessive thickness increases charge transport resistance this findings matches the research done by (Shrabni *et al*.,2017)

I-V Characteristics of $CUAlO_2$/ZnO and NiO/ZnO Perovskite Solar Cells

Figures 12 and 13 show the I-V characteristics for $CUAlO_2$/ZnO and NiO/ZnO perovskite solar cells respectively it could be observed that $CuAlO_2$/ZnO perovskite solar has slightly higher current density Jsc and Voc than NiO/ZnO leading to better overall efficiency and the overall efficiency drops with increasing thicknesses for both cases and this due to reduced charge transport and at the same time NiO/ZnO perovskite solar cell provides slightly better performance at lower thickness this findings matches with the results research done by (Ahmed *et al.,*2018) this is because NiO has higher hole mobility than $CuAlO_2$ leading to better charge extraction at thin layers and it exhibits more stable conductivity at thinner layers compared to $CuAlO_2$ (Anat, *et al*.,2022)

CONCLUSION

The numerical simulation of $CuAlO_2$/ZnO and NiO/ZnO-based perovskite solar cells has demonstrated the crucial role of temperature, layer thickness, and electrical properties in optimizing device performance. Through systematic variation of these parameters, notable improvements in key photovoltaic metrics were observed. For both $CuAlO_2$/ZnO and NiO/ZnO configurations, optimized absorber and transport layer thicknesses contributed to enhanced light absorption and efficient charge extraction. The $CuAlO_2$/ZnO

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structure achieved a higher open-circuit voltage (Voc) due to improved band alignment and reduced recombination losses, while the NiO/ZnO configuration displayed better short-circuit current density (Jsc), attributed to its superior hole transport capabilities. Simulations indicated that under optimal conditions: Voc values increased significantly, reaching up to ~1.1 V, Jsc improved to over 22 mA/cm²,Fill Factor (FF) exceeded 78% in the best cases, Leading to a Power Conversion Efficiency (PCE) enhancement, with maximum values approaching or surpassing 20%.Moreover, the effect of temperature variation highlighted the thermal sensitivity of perovskite materials, with performance degradation observed beyond certain temperature thresholds. $CuAlO_2$-based cells exhibited better thermal stability compared to NiO-based cells, suggesting their potential advantage in real-world applications. In conclusion, this study underscores the importance of optimizing structural and electrical parameters in perovskite solar cells. The findings provide a strong foundation for further experimental validation and development of high –efficiency, thermally stable perovskite photovoltaic devices.

REFERENCES

Achilease, S. Ioannis, T. P. Dimitris, T. Apostolos, I. Fedros, G. and Kontantinos, K. (2019) Inverted perovskite photovoltaics using flame spray pyrolisis solution based $CuAlO_2$/Cu-O hole – selective contact https://doi.org/10.1021/acsaem.9b00070

Ajay, K. Uddeshya, G. Tanya, T. and Neha, G (2020). Simulation of perovskite solar cell employing ZnO as an electron transport layer (ETL) for improved efficiency doi.org/10.1016/j.matpr.2020.07.267

Ahmed O. M.. Alzahrani M. S. Abdel-wahab, M. S. and Aida, M. S. (2018) Effect of ZnO layer thickness upon optoelectrical properties of NiO/ZnO heterojunction prepared at room temperature journal of materials science vol. 29 Pp 16317-16324

Akande F. Peter, O, Ayodeji, O. S. Abideen, A. (2023) SCAPS 3201 simulation of tunable heterostructured *p*-CdTe and n-CdS thin films-based solar cells

Aliyu, K. Nafarizal, N. and Ahmad, H. A. (2019). Chapter 6 Indium Tin Oxide thin films: An Ideal transparent and Conducting Oxides Contact for solar cells application. Optical fiber laser TECHNOLOGY Series 2 Pp 62 ISBN No:9789672389378

Amu T. L. (2014) Performance optimization of Tin Halide perovskite solar cells via numerical simulation Department of theoretical physics African University of Science and Technology, Abuja

Anat, I. Xu, H. Adi, K. Sujit, K. Michal, E. Antoine, k and David C. (2022). NiN-Passivated NiO HOLE- transport layer improves halide perovskite-based solar cells. ASB Publications doi:.org/10.1021/acsami.2c11701

Anselem, C. E. Eli, D. Rita, C. O. Nicholas, N. T. Christopher, U. A. Idoko, S. H. Loveth, O. E (2023) Defect and doping concentration study with series and shunt resistance influence on grapheme modified perovskite solar cell: A numerical investigation in SCAPS-ID framework 0019-4522 Indian chemical society https://doi.org/10.1016/j.jics.2023.10100,

Akanksha, S. Chougalea, C, Harshad, D. Shelkea, B. P, Sandesh, R. Jadkara, N. N, Habib M. P. and Dnyaneshwar R. Shinde (2022.) Simulation of P-CdTeandN-TiO2 Heterojunction Solar Cell EfficiencyVolume2Issue1

E-ISSN: 3115-4662 DOI: 10.64290/bima.v9i2B.1289

Arya K. and Subash, T.D. (2023). Simulation of NiOx Based Solar Cells Using SCAPS Software
NanoWorld Journal Research Article Open Access https://doi.org/10.17756/nwj.2023-s5-028

Bett, K. Kiprotich, S. Ungula, J. and Andayi, W. (2024) Structural and optical properties of ZnO : Al: Ga co-doped Nanoparticles: Investigation on the effects of pH of the precursor solution via a simple sol-gel route p-ISSN:2162-9382 14(2): 21-30 doi:10.5923/j.materials.20241402.01

Bhamu, K. C. Rhaba, K. Saleem, A. K. and Priolkar, K. R (2016) Electronic, Optical and Thermoelectric
properties of 2H-$CuAlO_2$: A first principles study. Journal of electronic materials 45(1):615 DOI: 10.1007/s11664-015-4160-3

Chufeng, Q. Yan, W. Jiaxing, S. Wentao, W. and Zaifang, L. (2022). Efficient planar perovskite solar cells with ZnO Eectron transport layer https://doi.org/10.3390/coatings12121981

Danladi, E. Dogo D.S. Michael, S.U. Uloko, F.O. Salawu, A.O. (2021) Recent advances in of modeling perovaskite solar cells using SCAPS-ID: Effect of absorber and ETM thickness,
East.Eur. J. phys 4 5-17 https://doi.org/10.26565/2312-4334-2021-4.01

Derbali, L. Bouhjar, F. and Derbali, B. M (2023). Enhenced ZnO-based ETL and nanostructured interface modification for improved perovskite solar cells efficiency
https://doi.org/10.1016/j.opmat.2023.114440

DiZhou , W. Tiantian Z. YuTian, X. Z, and Yafang T. (2018) Perovskite-Based Solar Cells: Materials, Methods, and Future Perspectives Hindawi Journal of Nanomaterials Volume 2018, Article ID 8148072, Pp15 https://doi.org/10.1155/2018/8148072

Dong, Y. Ruixia Y. Jing, Z. Zhou, Y. Shengzhong, L and Can, L.(2015). High efficiency flexible perovskite solar cells using superior low temperature TiO_2. Energy and Environmental science

Elfarri, H. Bouachri M, Frimane A, Fahoume M, Daoudi O, (2021). Optimization of simulations of thickness layers, temperature and defect density of CIS based solar cells, with SCAPS-1D software, for photovoltaic application. Chalcogenide Lett 18(4): 201-213. https://doi.
org/10.15251/cl.2021.184.201

Eli, D. Onimisi, M.Y. Garba, S. Gyuk, P. M. Jamila, T. and Boduku, H. P.(2020). Improved power conversion efficiency in perovskite solar cells using silver nanoparticles modified photoanode
Materials science and Engineering 805 (2020) 012005 doi:10.1088/1757-899X/805/1/012005

Emmanuel, A.N. Timothy, A. A. Eli, D. Christopher, E. A. and Patience, E. O (2024) Simulation and
Optimization of 30.17% high performance N-type TCO-free inverted perovskite solar cell using inorganic transport material https://doi.org/10.38/s41598-024-52882-7

Farhana, B. S. Muhammad, K. Eli, D. Ammar M. Tighezza, N A, Gazi, F. I. Toki, R. and Khalid H. M. (2023) Optimization of Perovskite-KSnI3 Solar Cell by Using Different Hole and
Electron Transport Layers: A Numerical SCAPS-1D Simulation
Cite This: Energy Fuels 37, 19207−19219

Femi, I. Meng, L. Yun, H. Liao, L. S. and Zhao-Kui, W. (2015) Room temperature

E-ISSN: 3115-4662 DOI: 10.64290/bima.v9i2B.1289

$CuAlO_2$ hole interfacial layer for efficient and stable planar perovskite solar cells. Journal of material chemistry A-4(4) DOI:10.1039/C5TA07957H

Gao, P. Gratzel, M. and Nazeeruddin, M .K. (2014) Organohalide lead perovskite for photovoltaic applications, Energy Eviron sci.7 2448-2463 https://doi.org/10.1039/C4EE00942H

Green, M. A. Ho-Baillie, A. and Smith, H. J. (2014). Fabrication of perovskite-Type photovoltaic devices with polysilane Hole transport layers https://doi.org/10.1038/nphoton.2014.134

Hussein. A. R. Samer. M. and Abdul A. (2024). Optimization of Thickness, Energy Band Gap, and Temperature for High Efficiency of Lead Halide Perovskite Solar Cell Int J. Thin Film Sci.Tec. 13, No. 3, 225-233 http://dx.doi.org/10.18576/ijtfst/130307

Hossain, M.K. Rubel, M.K.H. Toki, G.F.I. Alam, I. Rahman M. F. Bencherif, M. F. (2022). Effect of various electron and hole transport layers on the performance of $CsPbI_3$ BASED perovskite solar cells a numerical investigation in DFT, SCAPS-ID and wxAMPS framework

Hui-jing, D. Wei-Chao, W. and Yi-Fn, W. (2017) Simulation design of P-I-N-type all perovskite solar cells with high efficiency Chinese physics B, vol. 26, Number DOI:10.1088/1674-1056/26/2/028803

Jayan, D. K. and Sebstian, V. (2021) Comprehensive device modeling and performance analysis of $MASnI_3$ based perovskite solar cells with diverse ETM, HTM and back metal contacts https://doi.org/10.1016/j.solener.2021.01.058

Khalid, M. Hossain G. F. Ishraque, T, Abdul Kuddus, M. H. K. Rubel, M. M. Hossain, H. Bencherif, M. Ferdous Rahman, M. Rasidul Islam, 8. and Muhammad M. (2023). An extensive study on multiple ETL and HTL layers to design and simulation of high performance lead-free CsSnCl3-based perovskite solar cells, https://doi.org/10.1038/s41598-023-28506-2

Kurawa, S. M. Musa. A. O. Darma, T. H. Getso, R. S. and Bunkure, Y. I. (2022). Synthesis and Characterization of Zinc Oxide (ZnO) Thin Films for Solar Cell Applications Using Sol-Gel Auto Combustion Technique Journal of Materials Science Research and Reviews Volume 5, Issue 4, Page 475-482, 2022; Article noJMSRR.95374

Lin, L. Jiang, L. Qiu, Y. and Yu, Y (2017). Modeling and analysis of HTM-free perovskite solar cells based on ZnO electron transport layer https://doi.org/10.1016/j.spmi2017.02.028

Ligyan, L. Jiang, L. Q. Ping, L. and Yu, Q.(2019).Numerical modeling of inverted perovskite solar cell based on CZTSSe hole transport layer efficiency improvement. Journal of photonics for energy.9(03):1 DOI:101117/1.JPE.9.035501

Lwitiko, P. M. Lennart, L. Monika, R. Alexander, W. Ulrich, W. P. Bryce, S. R. and Michael, H. (2020). Impact of Silver incorporation at the back contact of Kesterite solar cells on structural and device properties. Thin solid film, Elsevier vol.209

Mandadapu, U. Victor, S. V. and Thyagarajan, K. (2017)Simulation and Analysis of Lead based Perovskite Solar Cell using SCAPS-1D Vol 10(11), DOI: 10.17485/ijst/2017 ISSN (Print) : 0974-6846

E-ISSN: 3115-4662 DOI: 10.64290/bima.v9i2B.1289

Mohammed, B. K., Ahmed-A. K. Abdelkrim, E. M. Souraya G. S.(2020).Device design optimization with interface engineering for highly efficient mixed cations and halides perovskite solar cells

Marlein, J. Burgelman M. (2007) Proceedings of NUMOS (Int. Workshop on Numerical Modelling of Thin Film Solar Cells, Gent (B), 28-30 March 2007). p. 227-233 2007,

Minbashi, M. Ghabadi, A. Ehsani, M. H. Rezaghalipour, H. and Dezaji, N. M. (2018) Simulation of high efficiency SnS-based solar cells with SCAPS. Solar energy vol. 176 Pp520-525

Pauwels, H.J. Vanhoutte, G. (2007) Influence of interface states and energy barriers on efficiency of heterojunction solar-cells, J. Phys. D-Appl. Phys., 11 649-667

Pradeepkumar, M. S. Sibin, K. P. Swain, N. Sridhara, N. Dey, A. Barshilia, H. C. and Sharma A. K. (2015) Nanoindentation response of ITO film https://doi.org/10.1016/j.ceramint.2015.02.090

Priyanka R, Numeshwar K. S. Ayush, K. (2020) An investigation on the impact of temperature variation over the performance of tin-based perovskite solar cell: A numerical simulation approach www.elsevier.com/locate/matpr

Rohan, G. Anterdipan, S. Pratima, A. (2022). Study on effect of different HTL and ETL materials on the perovskite solar cell performance with TCAD simulator,

Shrabni, P. Daiela, N. Tomas, C. Kasra, K. Rodrigo, M. Elvira, F.(2017). Oxide-based solar cell: Impact of layer thicknesses on the device performance. doi: 10. 1021/acscombsci.6b00154 Epub

Shasti, M. and Martezaali, A. (2019) Numerical simulation of Cu_2O , $SrCu_2,O_2$ and $CuAlO_2$ as hole transport materials for application in perovskite solar cells https://doi.org/10.1002/pssa.201900337

Suresh, K. M. and Chandra, B. k. (2021) A review on Solar cells (PSCs), materials and applications, science direct vol 7 issue 5

Takashi, E. and Takoyashi, N. (2016) Preparation of $CuAlO_2$ thhin film by sol-gel method using Nitrate solution Dip-coating DOI:10.1051/matecconf/20166704012

Tala-Ighil Zaïr, Oudjehani, R,.C. and Tighilt, K. (2021) SCAPS Simulation for Perovskite Solar Cell Journal of Solar Energy Research Updates, 2021, 8, 21-26

Wang, K. Xu, Z. Ling, F. Wang, Y. and Dong, S. (2019). Annealing and thickness effects on magnetic properties of ZnO and Co2FeAl alloy films Applied surface science vol435Pp 1125- 1135

Yang, Y Ngoc, D. P. Disheng, Y. Huaiyong, Z. Prasad, Y. and Hong, W.(2018). Inorganic p-type semiconductors and Carbon materials based hole transport materials for perovskite solar cells https://doi.org/10.1016/j.cclet.2018.05.008

Yu, Z. Ishanie, R. P. Torben, D. and Udo, B. (2016) Indium tin oxide as a semiconductor material in efficient p-type dye-sensitized solar cells 8(9):e305 DOI:10.1038/am.2016.89

Zhang, X.; Zhou, H.; Hu, C.; Zhao, Y.; Ma, X.; Wu, J.; Qi, Y.; Fang, W.; Jia, S.; Yu, J. (2023) Performance analysis of all-inorganic Cs3Sb2I9 perovskite solar cells with micro-offset energy level structure by SCAPS-1D simulation and First-principles calculation. Sol. Energy Mater. Sol. Cells 260, 112487.

Zioloa, R F. (2016). Inorganic Nanoparticles. In Llop J, Gomez-Vallejo V (eds)

E-ISSN: 3115-4662 DOI: 10.64290/bima.v9i2B.1289

Isotopes in Nanoparticles Fundamentals and Applications. Routledge.