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Conference paper

Optimizing Hybrid Perovskites for High-Efficiency Solar Energy

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ABSTRACT

Our research explores hybrid perovskite solar cells, promising low-cost and high-efficiency photovoltaic solutions. Despite challenges, optimizations like interface engineering enhance performance for future commercial use. Study of different physical parameters with the help of *SILVACO* and *MATLAB Simulink* for cell modeling. Long-term stability and cost reductions are among the most significant challenges to broad commercialization Future research will be around trying different parameter values. There searcher said this project represents an important step forward in the development of hybrid perovskite solar cells, which could be a key partof a new wave of clean energy sources that are needed as global consumption levels continue to rise. The solar cells studied herein are detailed by the six-scan structure: *Glass/Indium Tin Oxide (ITO) / Electron Transport Layer - (N layer) - Active Layer (Perovskite) - Hole transport_layer (Payer) - Metal Electrode; Glass/ITO/TiO2/Pero_Aardes Spiro-OMeTAD/Au*. It delivers the energy conversion efficiency of *19.12%* with a fill factor (*FF*) of *80.53%*, an open-circuit voltage at *Voc =1.14 V*andshort circuit current density *Jsc=20.88 mA/cm²*,respectively The active layer is a *0.25 µm*-thick *CH3NH3PbI3* perovskite, and the TiO2 layer thickness was set at *0.02 µm*

1. INTRODUCTION

Sustainable and renewable energy sources are required by the increasing global demand of energy, environmental concerns, and the finite supply of fossil fuels. Among available alternatives, solar energy seems to be the most promising option towards clean energy availability. Solar cell technology is able

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to directly convert photon energy into electricity there by creating a renewable, eco-friendly pathway for us to follow. In the last few decades, photovoltaic modules have become more affordable with time *(Nikolina, 2016; Abdelilah et al.2020; Huang, 2020; Franhofer & Energiewende, 2015; Energiewende, 2015; Bouab & Garn, 2022)*. Photovoltaic modules generated *821* terawatt-hours (*TWh*) of electricity globally in 2020 *(Jager-Waldau, 2023)*. At present silicon-based photovoltaic (*PV*) modules dominate the worldwide market mainly because of their superior power conversion efficiencies that can reachup to *26.7%* using mono crystalline silicon under laboratory conditions as well as their cost-effectiveness *(Dale & Scarpulla, 2023))*.

To implement solar cell technology globally, significant advancements in the materials and devices used are essential. These improvements are key to reducing manufacturing costs and increasing power conversion efficiency. Among the different types of third-generation solar cells, perovskite solar cells (PSCs) have experienced exceptional growth in recent years, recently achieving an efficiency of over 33.7%. Although perovskite solar cells have shown great potential, their lack of stability and the challenges associated with scaling up have hindered their path to commercialization.

Current research into PSCs mostly focuses on achieving high efficiency and stability through different fabrication methods, as well as material engineering. The recombination reactions have been essential for achieving high-performance *PSCs*. Moreover, environmental degradation of *PCE* remains a significant issue requiring serious attention.

The aim is to develop and simulate a wide-band gap perovskite solar cell using *Tcad Silvaco* in this paper, optimize it with a single-cation perovskite and analyze both the solar cell itself and the materials used.

2. MATERIALS AND METHODS

In order to boost the performance of Perovskite-based solar cells, we simulated a structured cell *Glass/Indium Tin Oxide (ITO)/Electron Transport Layer (ETL)/Active Layer (Perovskite)/Hole Transport Layer (HTL)/Metal Electrode*: *Glass/ITO/TiO2/Perovskite/Spiro-OMeTAd/Au* in Figure *1* by changing several parameters.

Firstly, we selected one reference cell containing a set of fixed values to simulate the effect of different parameters. Following that, one parameter was changed at a time while keeping others constant in order to study how they affect the properties of the Tandem Perovskite cell. The structure of the reference cell used in simulation is presented in figure 1.

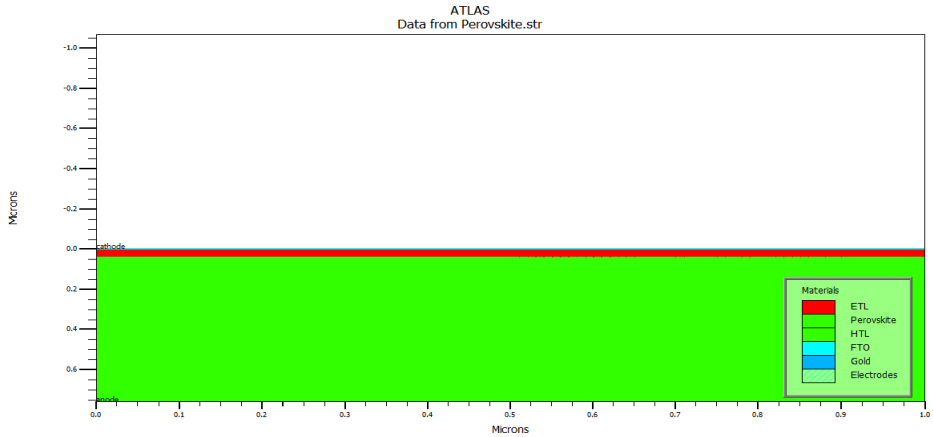

Figure 1. Structure of the reference cell.

2.1 Parameters of the simulated structure

The parameters of the reference cell are illustrated in the following table

Tab.1.2.Parameters of the reference cell

	Thikness (µm)	**Concentration (cm^3)**	**Eg (eV)**
TiO_2	*0.02*	*$Na=1.10^{19}$*	*3.20*
Pérovskite	*0.54*	*$Nd=1.10^{15}$*	*1.60*
Spiro	*0.2*	*$Nd=1.10^{19}$*	*2.6*

To perform a numerical simulation, it will be necessary to establish the structure's mesh. *Deckbuild* tool is used to describe doped regions (position, type, concentration and doping profile), create electrical contacts on the structure and define the mesh.

The mesh subdivides the simulated structure into small cells for solving numerically continuity equation, Poisson equation and current density equation. For this reason, for a highly precise simulation its mesh should be very fine. Nonetheless, a very fine mesh results in a large number of elements that need to be computed hence they take too much time during calculation. Consequently, there is need for compromise between accuracy of calculations and time available. The defining of the Mesh helped us obtain all electric parameters of reference solar cell including *AM1.5* solar spectrum. Figure 2 shows solar cell structure with three main regions required by SILVACO-ATLAS when more elements are computed. Figures 9 and *10* present these findings.

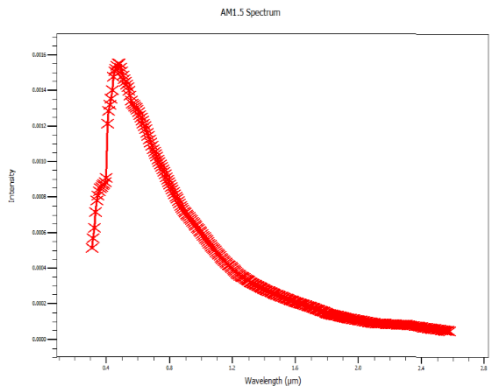

Figure 2. The solar spectrum used AM1.5

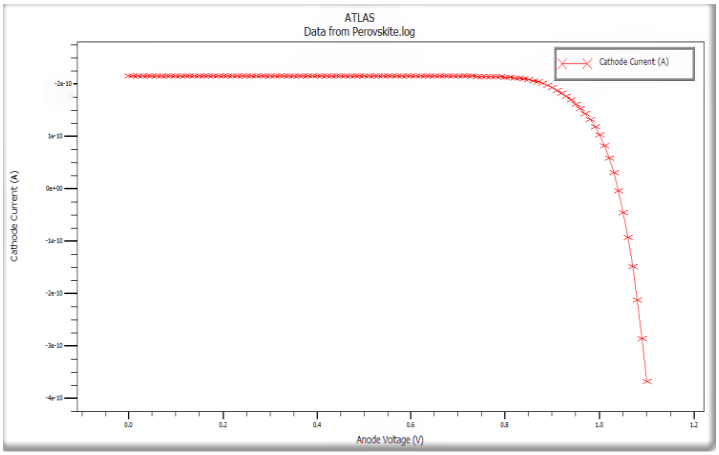

Figure 3. I-V characteristic of the reference perovskite-based solar cell

3. RESULTS AND DISCUSSION

3.1 Thickness parameters

We adjusted the thickness of the acceptor layers, while keeping everything else the same. The results of these adjustments are shown in the following figures.

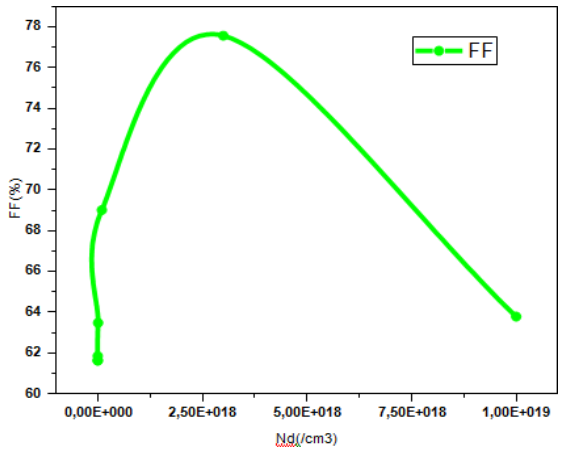

Figure 4. FF as a function of region thickness 1

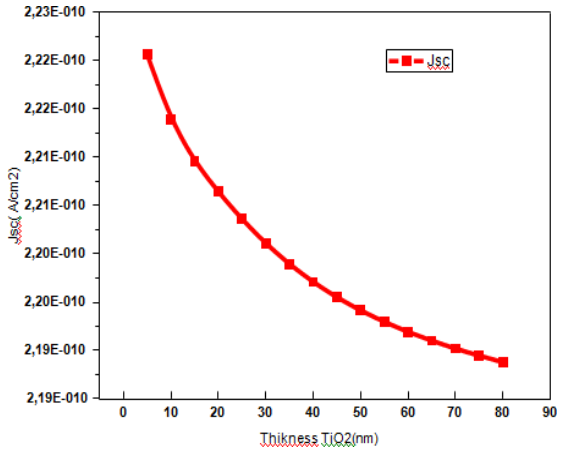

Figure 5. Jsc as a function of region 1 thickness

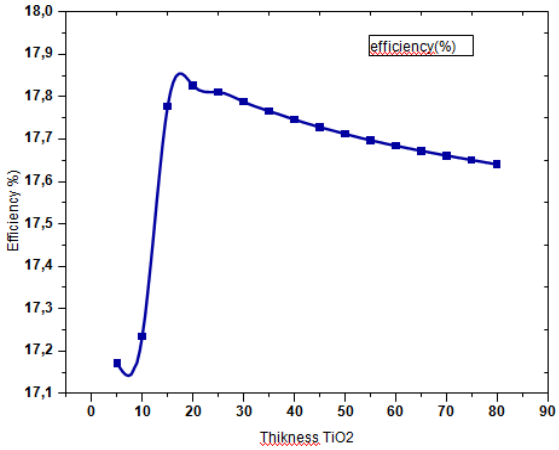

Figure 6.Yield as a function of region thickness1

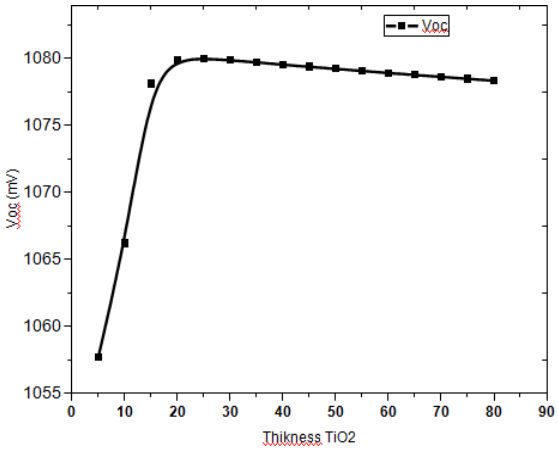

Figure 7. Voc as a function of region thickness1

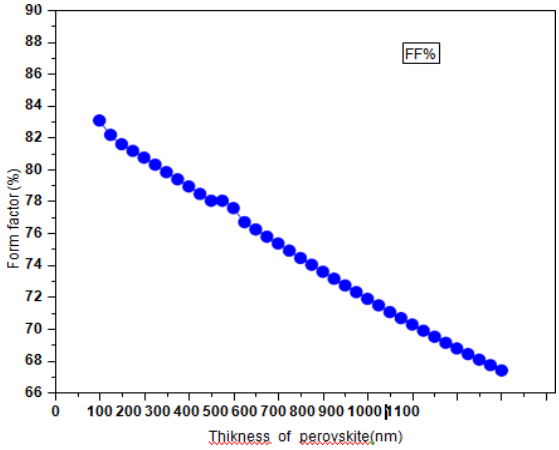

Figure 8. FF as a function of region 2 thickness

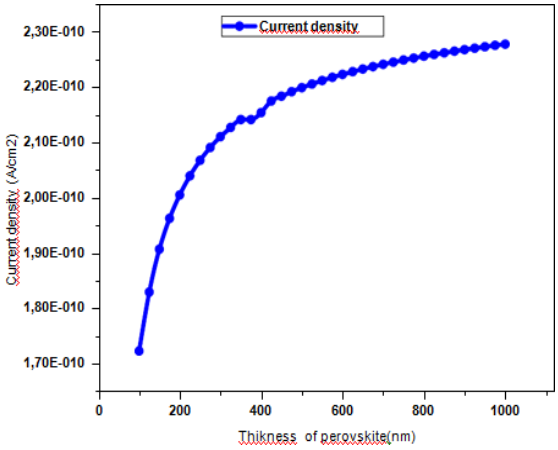

Figure 9. Jsc as a function of region2 thickness

3.2 Results of numerical simulation with SILVACO-ATLAS of Spiro OMED

With a spire layer thickness of *0.3µm*, we achieved optimal electrical parameters: an efficiency (η) of17.8298%, a fill factor (*FF*) of *74.7278%*, a short-circuit current density (*Jsc*) of 22.0935 *mA/cm²*, and an open-circuit voltage (*Voc*) of *1079.94 mV*. Optimizing the perovskite-based solar cell involves selecting the best parameters for each layer, based on these optimal electrical values, and then in putting them into the simulation program to obtain an optimized solar cell.

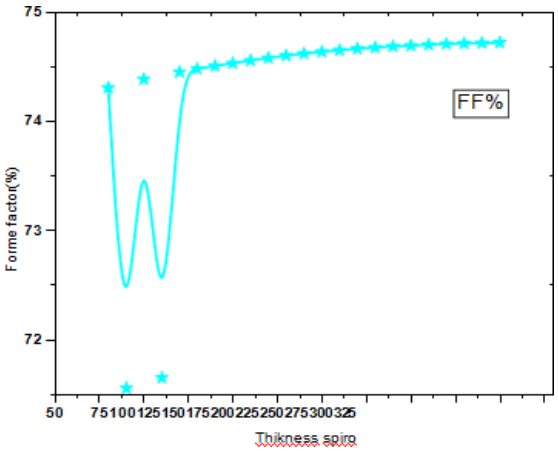

Figure 10. FF as function of region 3 thickness

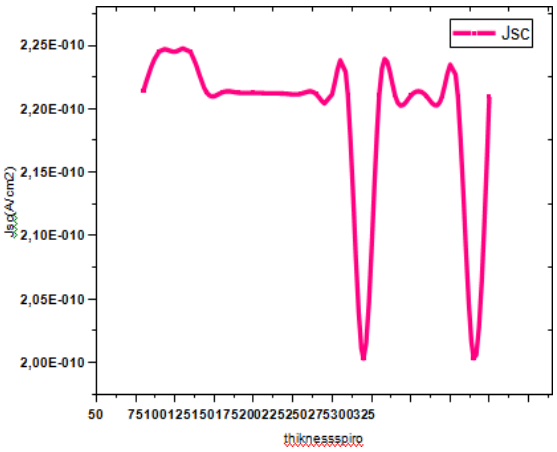

Figure 11. Jsc as a function of region thickness3

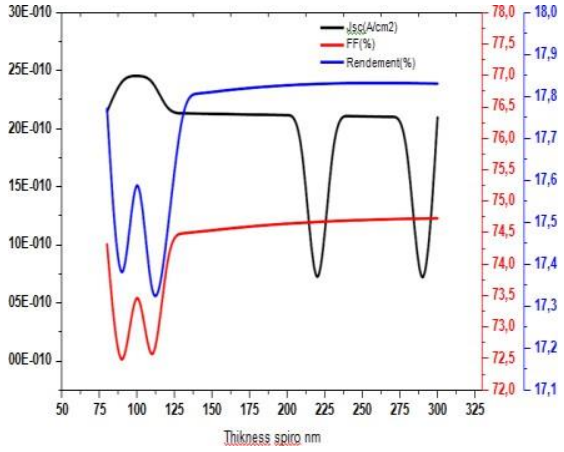

Figure 12. FF, Yield,Jsc as a function of region thickness 3

3.2.1 from Solar Cell to Photovoltaic Solar Panel Using MATLAB Simulink

In our study, we used a photovoltaic solar cell with a surface area of *1 µm²* in the *Tcad Silvaco* simulation. Typically, a mini photovoltaic solar panel measures *1.5cmx5cm*, which equals a surface area of *7.5cm² (Bouab & Garn, 2022)*. Let's consider a solar panel with these specifications:

- Open-circuit voltage:*22.3V*
- Short-circuit current :*1.13 A*

From this, we derived the following electrical values for the perovskite solar cell:

- Short-circuit current (*Isc*):*2.0883x10⁻¹⁰A*
- Open-circuit voltage(*Voc*):*1.13679 V*

To reach voltage of *22.3V* (*Voc*), we need to connect *20* solar cells in series. To achieve a current of *1.13A* (*Isc*), we need about *6.109* parallel circuits, each with *20* solar cells connected in series.

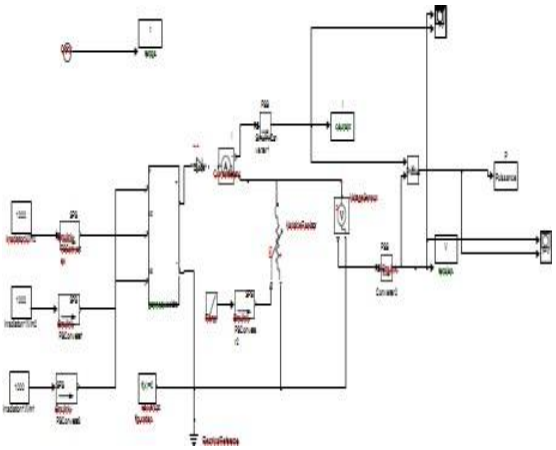

Figure 13. Matlab simulink representation of the solar panel

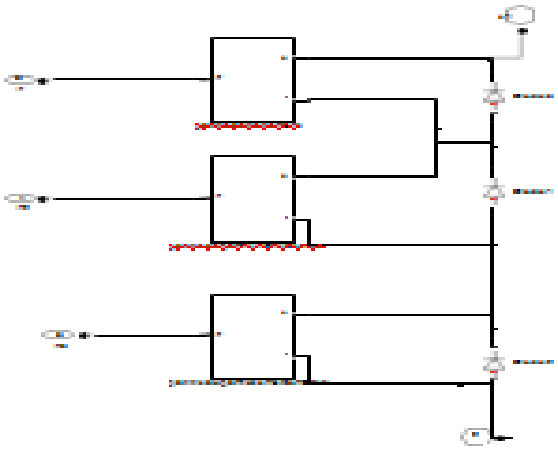

Figure 14. Representation of the three solar panels in series I as a function of irradiation at constant temperature

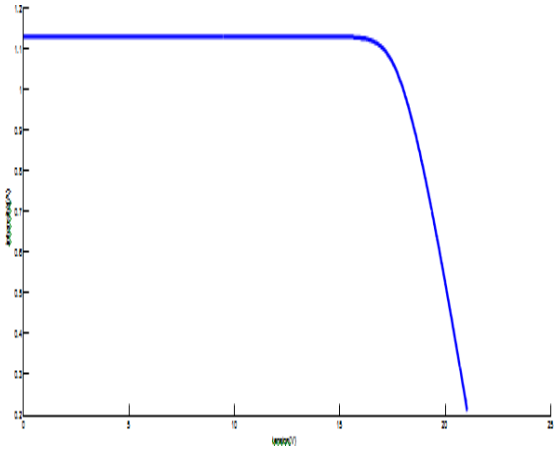

Figure 15. I-V characteristic of the Perovskite solar panel

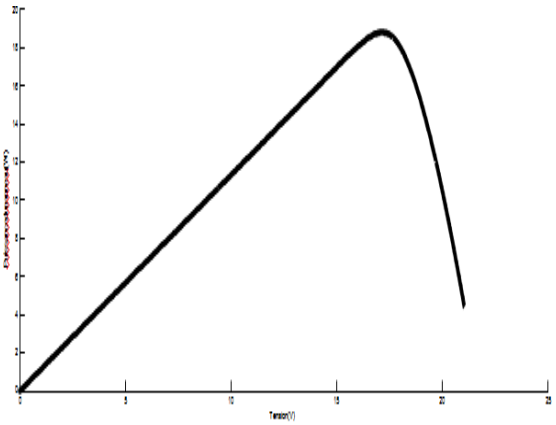

Figure 16. P-V characteristic of the perovskite-based solar panel

4. CONCLUSION

Our study on hybrid perovskite-based solar cells reveals their promising potential for photovoltaic conversion. Despite their high efficiency and lack of hysteresis, challenges remain with stability and reproducibility. We investigated various strategies to address these issues, including interface engineering and optimizing charge transport layers. Our simulations identified optimal configurations, achieving efficiencies over 19%. However, ongoing research is crucial for commercial integration and large-scale adoption. Moving forward, we plan to explore additional physical parameters and continue our efforts to enhance the stability and competitiveness of these solar cells in the global renewable energy market.

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