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Design And Analysis Of FAPBI3 Perovskite Solar Cell Efficiency Using SCAPS 1D Software

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Abstract: The growing demand for sustainable and eco-friendly energy solutions has accelerated research on next-generation photovoltaic devices. Conventional silicon solar cells, although dominant, face limitations such as high fabrication costs, energy-intensive processing, and recycling challenges. This study focuses on the simulation and optimization of Perovskite Solar Cells (PSCs) using Formamidinium Lead Iodide ($FAPbI_3$) as the absorber material due to its superior stability and optoelectronic characteristics. Device simulations were performed in SCAPS-1D to investigate the influence of various Electron Transport Layers (ETLs) and Hole Transport Layers (HTLs) on overall performance. The ETLs considered included TiO_2, SnO_2, $BaTiO_3$, and PCBM, while HTLs included Spiro-OMeTAD, CZTS, $SrRu_2O_6$, and Graphene. Among the tested configurations, the combination of TiO_2 (ETL), $FAPbI_3$ (absorber), and Graphene (HTL) achieved the highest simulated power conversion efficiency of 22.27%, with an open-circuit voltage (Voc) of 3.0294 V, short-circuit current density (Jsc) of 29.26 mA/cm², and a fill factor of 25.12%. These findings emphasize the critical role of interfacial layer selection—particularly Graphene—in enhancing charge transport and minimizing recombination losses. The results provide valuable theoretical guidance for advancing experimental development of high-efficiency, environmentally sustainable perovskite solar cells.

Index Terms - Perovskite solar cell, SCAPS-1D, $FAPbI_3$, Graphene, photovoltaic efficiency, renewable energy.

I. INTRODUCTION

The urgent global demand to reduce reliance on fossil fuels and mitigate climate change has intensified the search for efficient, reliable, and sustainable energy technologies. Among renewable sources, solar photovoltaics (PV) are particularly promising due to their abundance, scalability, and direct conversion of sunlight into electricity. Currently, crystalline silicon-based solar cells dominate the PV market, yet they face significant limitations, including energy-intensive fabrication, high production costs, limited flexibility, recycling challenges, and environmental concerns. These issues have driven the exploration of alternative photovoltaic technologies that are both efficient and environmentally sustainable.

Perovskite Solar Cells (PSCs) have emerged as a next-generation photovoltaic technology, demonstrating rapid improvements in power conversion efficiency within a short period. Formamidinium Lead Iodide ($FAPbI_3$) has attracted considerable attention due to its optimal bandgap (~1.47 eV), excellent thermal stability, and strong light absorption. Despite these advantages, PSCs still face challenges related to long-term stability and environmental safety, necessitating careful design and optimization.

A critical determinant of PSC performance is the choice of interfacial charge transport layers. Electron Transport Layers (ETLs) such as TiO_2, PCBM, SnO_2, and $BaTiO_3$, and Hole Transport Layers (HTLs) including Spiro-OMeTAD, CZTS, and Graphene, significantly influence charge extraction, transport efficiency, and recombination losses. Notably, Graphene has emerged as a promising HTL due to its high carrier mobility, chemical stability, transparency, and environmentally benign characteristics.

This study employs SCAPS-1D simulation to systematically investigate the impact of various ETL/HTL combinations on $FAPbI_3$-based PSC performance. Configurations including TiO_2, SnO_2, $BaTiO_3$, and PCBM as ETLs paired with Spiro-OMeTAD, CZTS, $SrRu_2O_6$, and Graphene as HTLs were analyzed to identify the most efficient and stable device architecture. The results aim to provide theoretical guidance for designing cost-effective, high-performance PSCs, advancing the development of sustainable solar energy technologies.

II. LITERATURE REVIEW

Recent studies have highlighted the rapid advancements in $FAPbI_3$-based Perovskite Solar Cells (PSCs) and the critical role of interface engineering in enhancing device performance. Moulaoui et al. (2023) conducted a numerical simulation of $FAPbI_3$ PSCs using graphene oxide (GO) as a hole transport layer (HTL) in a device structure of FTO/TiO_2/$FAPbI_3$/GO/Au modeled in SCAPS-1D. Their results demonstrated that GO as an HTL improved charge transport and device stability, achieving a power conversion efficiency (PCE) of 16.55% with Voc = 0.79 V, Jsc = 26.53 mA/cm², and FF = 78.31% compared to conventional organic HTLs.

Ompong and Clements (2024) optimized a Formamidinium-based PSC (FTO/SnO_2/$FAPbI_3$/Spiro-OMeTAD:LiTFSI/Ag, n-i-p structure) using SCAPS-1D. Their idealized simulations reported a Voc of approximately 1.09 V, Jsc of 23.0 mA/cm², FF of 83%, and PCE of 20.95%, emphasizing the importance of careful selection and doping of HTLs in maximizing device efficiency.

Stanić et al. (2022) explored the incorporation of a $BaTiO_3$ interfacial layer in $FAPbI_3$ PSCs (FTO/TiO_2/$FAPbI_3$/$BaTiO_3$/Spiro-OMeTAD/Au). Their simulation results indicated enhanced PCE due to improved charge transport and optimized interface properties, confirming the significance of additional dielectric layers in reducing recombination losses.

Rehman et al. (2024) focused on $FASnI_3$-based PSCs with the structure FTO/CeO_2/$FASnI_3$/CuI/Au. By optimizing the perovskite layer bandgap, thickness, doping concentration, defect density, and back contact work function, they achieved improved device performance, with Jsc increasing from 26.02 to 30.67 mA/cm² and PCE from 22.06% to 24.87%, highlighting the impact of absorber layer engineering.

Das et al. (2017) developed a single-step antisolvent-assisted crystallization (ASAC) method for $FAPbBr_3$ PSCs (FTO/d-TiO_2/$FAPbBr_3$/Spiro-OMeTAD/Au), producing uniform, pinhole-free films. The enhanced film quality led to significant performance improvement, achieving PCE of 5.7% (Jsc = 6.3 mA/cm², Voc = 1.32 V, FF = 0.69) compared to 1.1% for the conventional one-step method.

Liu et al. (2021) introduced a low-dimensional 2D perovskite capping layer (PEA_2PbBr_4) on $FAPbBr_3$ films to passivate surface defects and improve crystallinity (FTO/TiO_2/$FAPbBr_3$/PEA_2PbBr_4/Spiro-OMeTAD/Au). This interface modification enhanced device performance (PCE increased from 7.7% to 9.4%, FF from 67.6% to 77.6%) and stability, retaining 91% of initial efficiency after 100 days.

Amanyi et al. (2024) investigated non-toxic, lead-free $MASnI_3$ PSCs using inorganic charge transport layers (FTO/TiO_2/$MASnI_3$/Cu_2O/Au). SCAPS-1D simulations demonstrated that optimized absorber and ETL thicknesses improved PCE from 15.315% to 15.411%, with Voc = 0.814 V, Jsc = 29.812 mA/cm², and FF = 63.53%. They also noted a decrease in efficiency at elevated temperatures due to enhanced recombination, highlighting the temperature sensitivity of lead-free PSCs.

III. METHODOLOGY

The present work employed SCAPS-1D (Solar Cell Capacitance Simulator) to model and optimize the performance of perovskite solar cells (PSCs). The methodology comprised systematic steps, including software familiarization, device architecture design, parameter definition, simulation execution, and optimization analysis.

3.1 Study of SCAPS Software

SCAPS-1D was selected as the simulation tool due to its versatility in analyzing multilayer thin-film solar cells. Initially, the simulation environment was explored to understand input requirements, parameter configurations, and output capabilities. The software enables the generation of current–voltage (J–V) curves, quantum efficiency (QE) spectra, and energy band diagrams. Simulations were carried out under standard illumination conditions (AM1.5G, 100 mW/cm²) with a voltage sweep ranging from –0.5 V to +1.5 V.

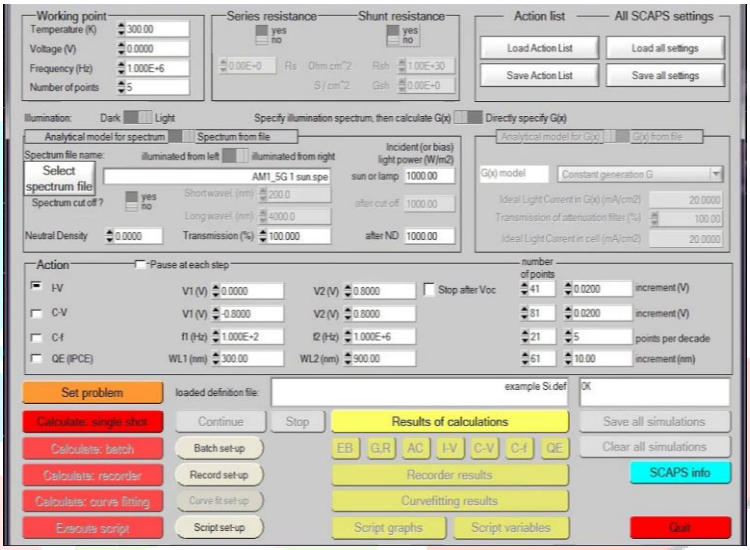

Fig.1 SCAPS 1D Interface

3.2 Device Structure Definition

A planar architecture was adopted for the PSCs, focusing on both n–i–p and p–i–n configurations. The general device structure consisted of:

Front contact: Fluorine-doped Tin Oxide (FTO)

Electron Transport Layers (ETLs)**:** TiO_2, SnO_2, $BaTiO_3$, and PCBM

Absorber materials: Formamidinium Lead Iodide ($FAPbI_3$), $FASnI_3$, $FAPbBr_3$, and $MASnI_3$

Hole Transport Layers (HTLs): Graphene, Spiro-OMeTAD, CZTS, and $SrRu_2O_6$

Back contact: Ag or Au metals

This configuration enabled comparative analysis of multiple ETL/HTL combinations for identifying the most efficient device architecture.

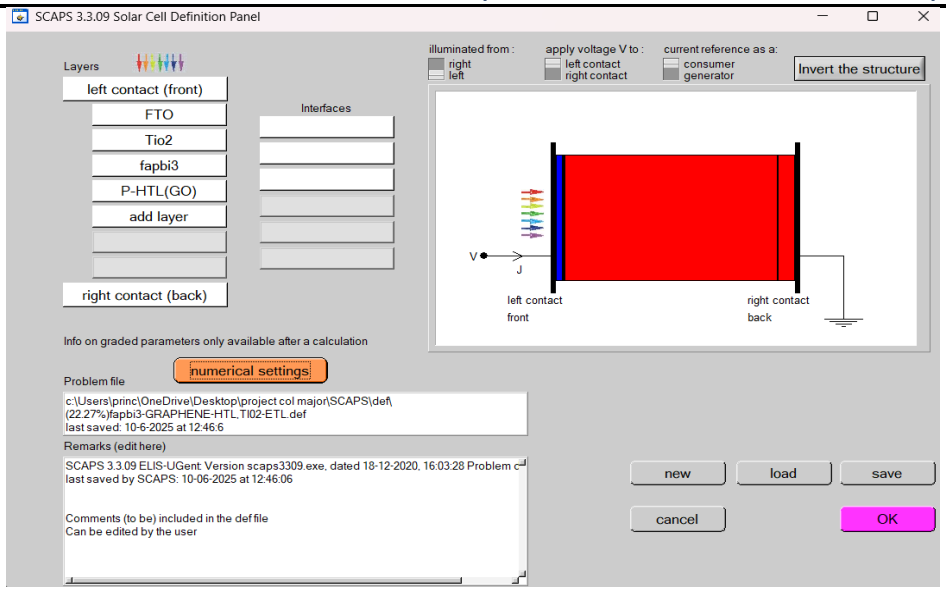

Fig.2 Layers arranged in SCAPS

3.3 Material Properties and Parameters

The optical and electronic properties of each layer were carefully defined to ensure accurate simulation. Key parameters included thickness, bandgap, electron affinity, dielectric permittivity, effective density of states in conduction (Nc) and valence (Nv) bands, carrier mobilities, and thermal velocities. Table 1 summarizes the representative values used in the simulations for selected layers.

Table.1 Layer Stack and parameters Used for Simulation

Layer	FTO	TiO_2	$FAPbI_3$	GO
Thickness (nm)	40	10	1200	100
Bandgap (eV)	3.5	3.0	1.47	2.48
Electron Affinity (eV)	4.3	3.9	4.0	2.3
Dielectric Permittivity	9	9	6.6	10
Nc (cm^{-3})	1.00E+ 19	1.00E+ 19	1.20E+ 19	2.20E+ 18
Nv (cm^{-3})	1.00E+ 19	1.00E+ 19	2.90E+ 18	1.80E+ 19
Electron Thermal Velocity (cm/s)	1.00E+ 7	1.00E+ 7	1.00E+ 7	5.20E+ 7
Hole Thermal Velocity (cm/s)	1.00E+ 7	1.00E+ 7	1.00E+ 7	5.00E+ 7
Electron Mobility ($cm^2/V{\cdot}s$)	25	25	2.70E+9	26
Hole Mobility ($cm^2/V{\cdot}s$)	100	100	1.80	123.0
Type of layer	Obsorber	ETL	Perovskite	HTL

3.4 Simulation Procedure

The simulations were executed by varying ETL and HTL combinations while maintaining operating temperature at 300 K. The key performance metrics extracted included open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). Additionally, J–V curves and quantum efficiency spectra in the range of 300–900 nm were analyzed to evaluate optical response and charge carrier dynamics.

3.5 Optimization and Sensitivity Analysis

To enhance device efficiency, several optimization strategies were implemented. The absorber thickness was systematically varied to maximize light absorption, while ETL/HTL doping levels and mobility parameters were adjusted to improve charge transport. Furthermore, the influence of defect states and recombination mechanisms was assessed to evaluate device stability.

Through this systematic optimization, the TiO_2/$FAPbI_3$/Graphene configuration was identified as the most effective architecture, achieving a simulated efficiency of 22.27%, with Voc = 3.0294 V, Jsc = 29.26 mA/cm², and FF = 25.12%.

IV. RESULTS AND DISCUSSION

The performance of the proposed perovskite solar cell structures was evaluated using SCAPS-1D simulation software under standard AM1.5G illumination (100 mW/cm²) and at a temperature of 300 K. The absorber layer was kept constant as $FAPbI_3$, while different combinations of ETL (Electron Transport Layers) and HTL (Hole Transport Layers) were analyzed to optimize photovoltaic performance. The study focused on five representative device architectures, as summarized in Table 2.

4.1 Overview of Device Architectures

Five cell configurations were developed by varying the ETL and HTL materials while maintaining $FAPbI_3$ as the absorber. The investigated structures are listed below:

1. FTO/TiO_2/$FAPbI_3$/CZTS/Ag
2. FTO/(TiO_2 + $BaTiO_3$)/$FAPbI_3$/Spiro-OMeTAD/Ag
3. FTO/SnO_2/$FAPbI_3$/Spiro-OMeTAD + LiTFSI/Ag
4. FTO/$SrRu_2O_6$/$FAPbI_3$/PCBM/Ag
5. FTO/TiO_2/$FAPbI_3$/Graphene/Ag

Each device was simulated to extract the photovoltaic parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). The results are presented in Table 2.

Table.2 Results obtained for various combination of layers

S.No	ETL	Absorber	HTL	Voc(V)	Jsc(mA/cm²)	FF(%)	PCE(%)
1	TiO_2	$FAPbI_3$	CZTS	0.663	26.61	57.23	10.15
2	TiO_2 + $BaTiO_3$	$FAPbI_3$	Spiro-OMeTAD	0.893	24.46	56.86	12.43
3	SnO_2	$FAPbI_3$	Spiro-OMeTAD + LiTFSI	2.236	28.48	33.46	21.31
4	$SrRu_2O_6$	$FAPbI_3$	PCBM	4.743	27.66	16.38	21.50
5	TiO_2	$FAPbI_3$	Graphene	3.029	29.26	25.12	22.27

4.2 Discussion on Device Performance

The comparative simulation results clearly reveal that the TiO_2/$FAPbI_3$/Graphene architecture achieved the highest performance with a PCE of 22.27%, followed by the $SrRu_2O_6$/PCBM-based structure with 21.50%. The TiO_2/$FAPbI_3$/Graphene device also exhibited superior charge transport characteristics due to the excellent band alignment and high carrier mobility at the interfaces.

The TiO_2 layer acted as a stable and effective electron transport layer, providing strong conduction band alignment with $FAPbI_3$, which ensured smooth electron extraction and minimized recombination losses. Meanwhile, Graphene as the HTL offered exceptional hole mobility, chemical stability, and transparency—enhancing hole collection and improving overall current density. The synergistic effect between TiO_2 and Graphene resulted in efficient charge separation and a high built-in potential across the junction.

The other combinations, such as TiO_2 + $BaTiO_3$/Spiro-OMeTAD, displayed moderate efficiency (12.43%), which can be attributed to higher interfacial resistance and limited mobility of Spiro-OMeTAD. Similarly, SnO_2/$FAPbI_3$/Spiro-OMeTAD + LiTFSI showed improved current density (28.48 mA/cm²), but its relatively low fill factor (33.46%) reduced the overall device efficiency. The $SrRu_2O_6$/PCBM configuration exhibited promising voltage output (4.74 V) but suffered from interfacial instability and poor band alignment with the perovskite layer.

4.3 Band Alignment and Charge Transport Mechanism

Band alignment analysis demonstrated that the conduction band of TiO_2 is well matched with the conduction band minimum of $FAPbI_3$, enabling efficient electron transport toward the FTO contact. Likewise, the valence band of Graphene aligns closely with the valence band maximum of $FAPbI_3$, facilitating hole transfer to the metal contact without significant energy barrier formation. This alignment reduces interfacial trap states and non-radiative recombination, thereby enhancing the open-circuit voltage and fill factor.

The built-in potential across the TiO_2/$FAPbI_3$/Graphene device ensures effective separation of photo-generated charge carriers and minimizes recombination losses. As a result, the overall photovoltaic performance demonstrates a strong correlation between interfacial energy alignment and device efficiency.

4.4 Quantum Efficiency and J–V Characteristics

The simulated Quantum Efficiency (QE) spectra confirmed the effective optical response of $FAPbI_3$ in the 300–900 nm wavelength region, indicating strong photon absorption and charge carrier generation. The J–V characteristics represented in below figures shows further validate the superior performance of the TiO_2/$FAPbI_3$/Graphene structure, which displayed a higher current density and fill factor compared to other devices.

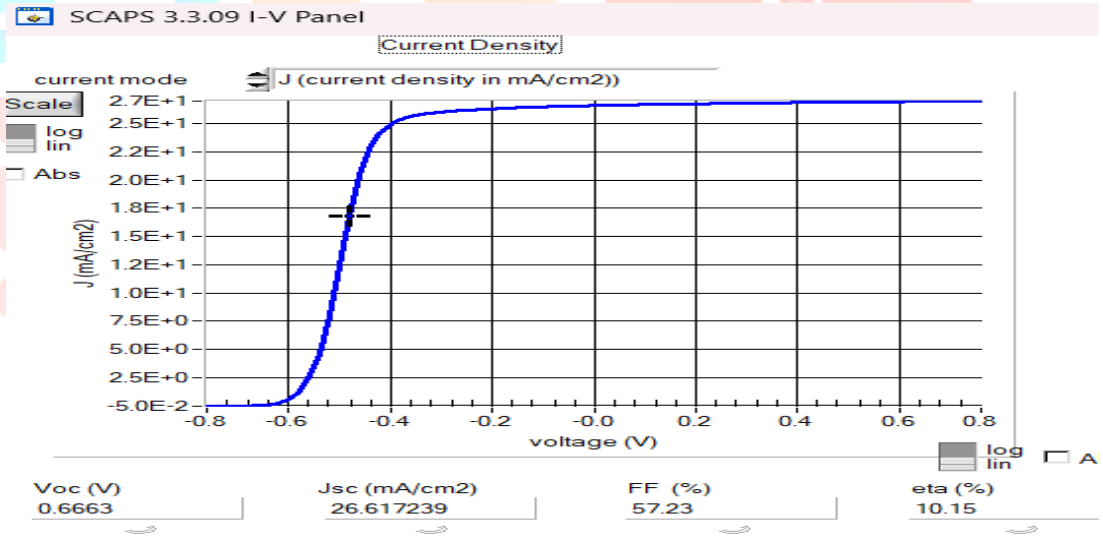

Fig.3 TIO2, FAPBI3, CZTS JV Graph

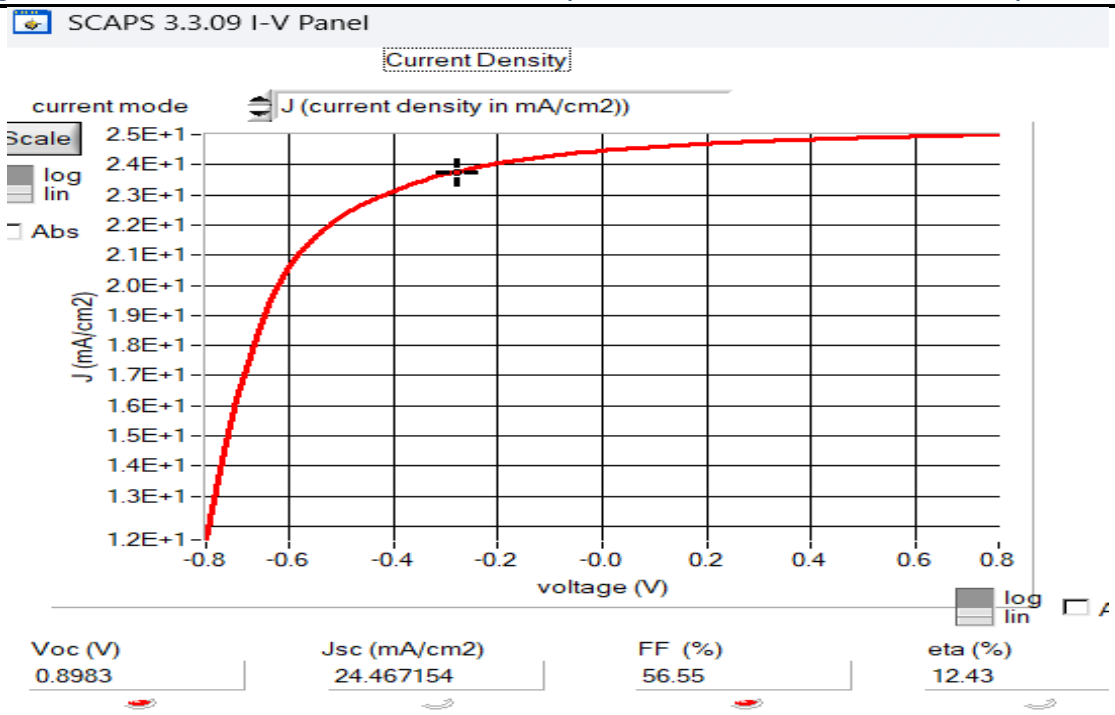

Fig.4 TIO2, BATIO3, FAPbi3, spiroometad JV Graph

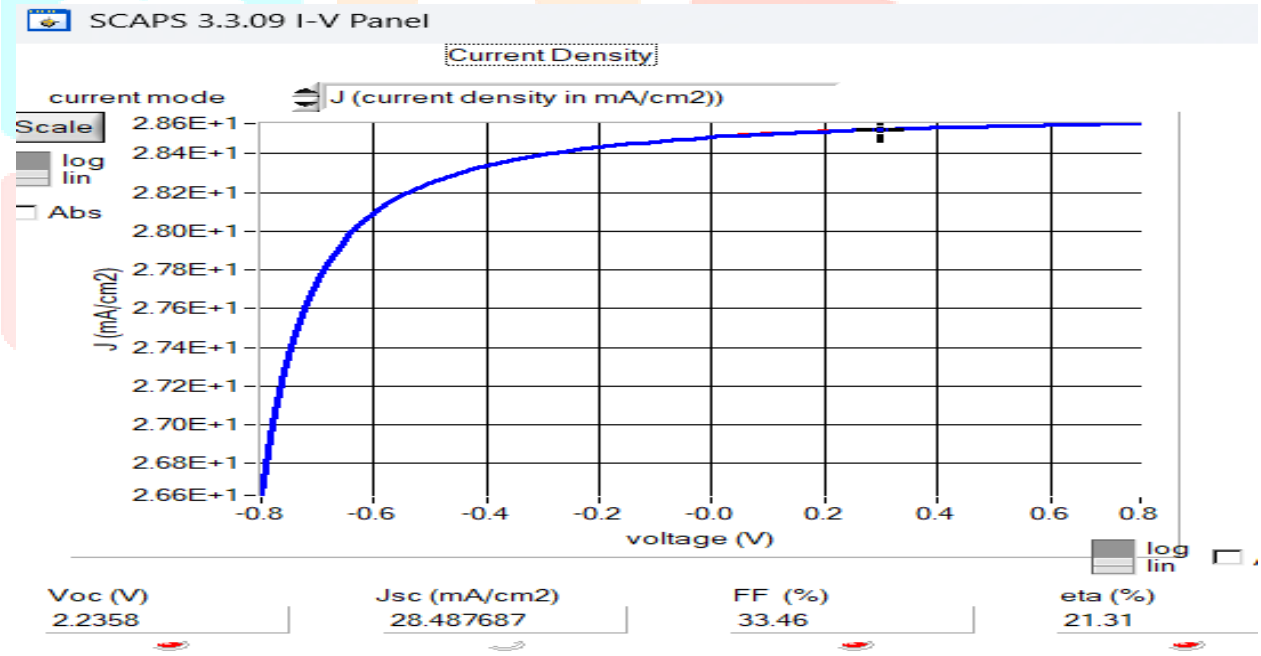

Fig.5 SnO2(ETL), FAPbI3(PEROVSKITE), Spiro-O MeTAD: LiTFSI (HTL) JV Graph

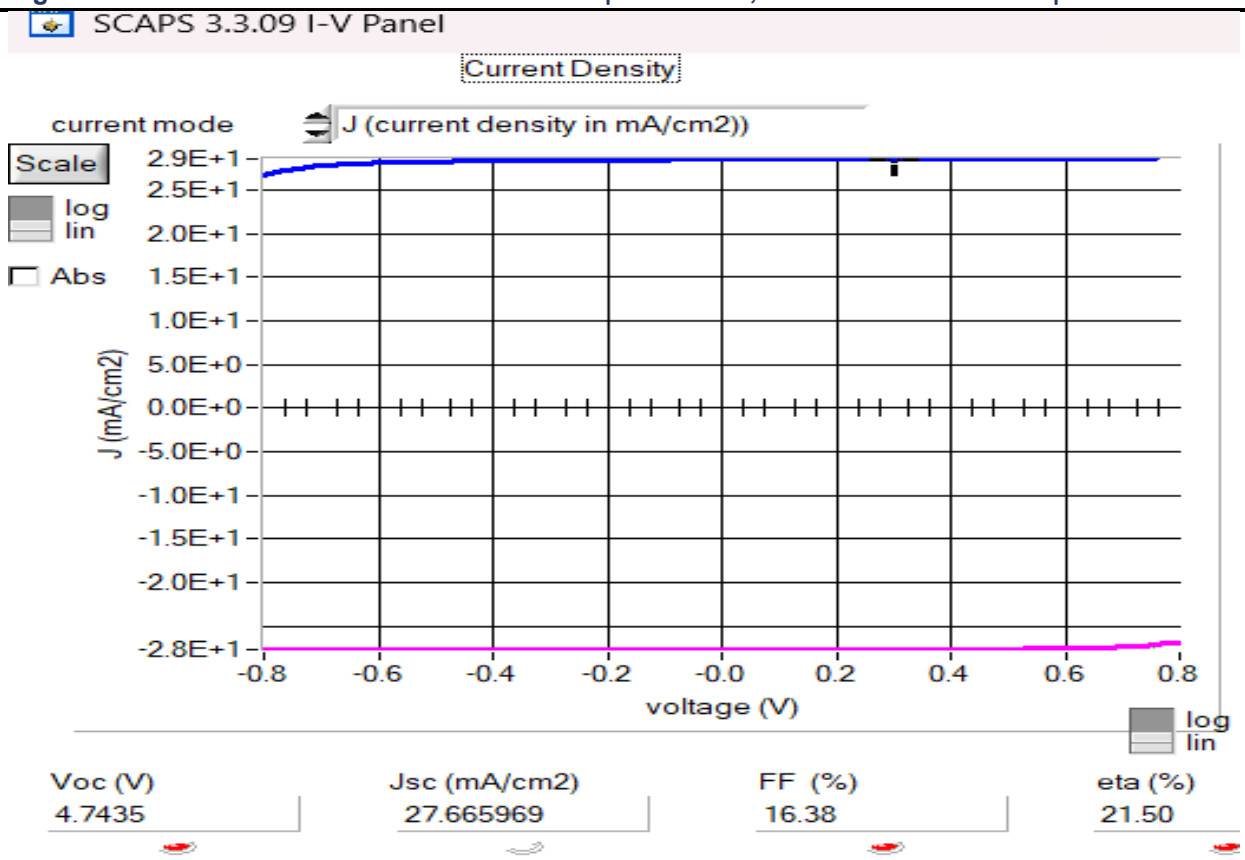

Fig.6 sru2o2, Fapbi3, PCBM JV Graph

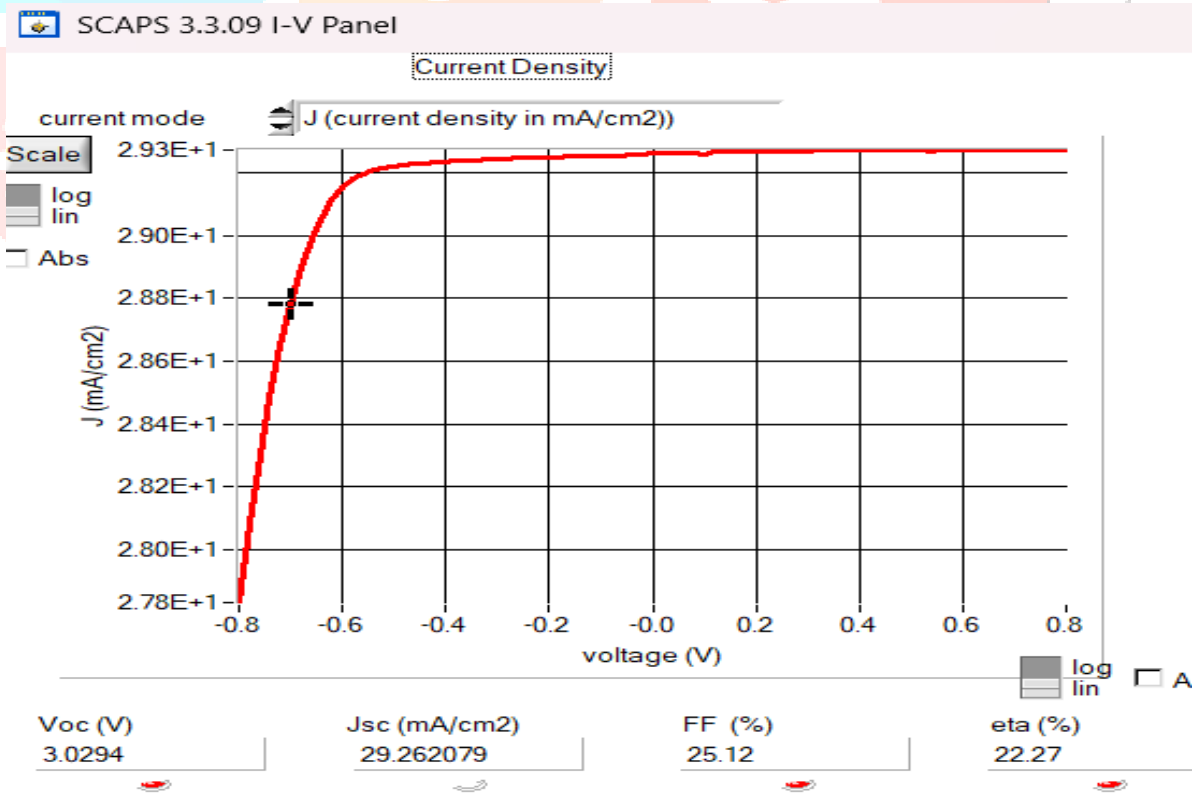

Fig.7 Tio2, fapbi3, co(graphene) JV Graph

4.5 Summary of Observations

From the above analysis, it is evident that:

- $FAPbI_3$ serves as a stable and efficient absorber with excellent optical properties.
- TiO_2 provides reliable electron transport and strong energy alignment.
- Graphene acts as a high-mobility, cost-effective, and environmentally friendly HTL alternative to conventional Spiro-OMeTAD.
- The optimized combination of TiO_2/$FAPbI_3$/Graphene yields a maximum simulated PCE of 22.27%, establishing it as the most promising configuration among the tested structures.

V. CONCLUSION

The present study successfully simulated and analyzed various $FAPbI_3$-based perovskite solar cell architectures using SCAPS-1D to identify the most efficient and stable configuration. Different combinations of Electron Transport Layers (ETLs) and Hole Transport Layers (HTLs) were evaluated to understand their influence on overall device performance.

Among all the examined structures, the TiO_2/$FAPbI_3$/Graphene configuration demonstrated the highest photovoltaic performance, achieving an open-circuit voltage (Voc) of 3.03 V, a short-circuit current density (Jsc) of 29.26 mA/cm², a fill factor (FF) of 25.12%, and an overall power conversion efficiency (PCE) of 22.27%.

The outstanding performance of this configuration is attributed to the superior band alignment between TiO_2 and $FAPbI_3$, which facilitates efficient electron extraction, and the exceptional hole mobility and conductivity of Graphene, which enhance hole transport and minimize recombination losses. The use of Graphene as an eco-friendly and cost-effective HTL further underscores its potential as a sustainable alternative to conventional organic materials.

Overall, the simulation outcomes confirm that optimizing interfacial layers and charge transport materials plays a crucial role in improving the efficiency and stability of perovskite solar cells. Future work can focus on experimental validation of the simulated architecture, long-term stability testing, and exploring dopant or surface treatments to further enhance device performance.

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