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ARTICLE

A hybrid machine learning and SCAPS 1D expedition for optimization of lead-free BeSiP₂ perovskite solar cells

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ABSTRACT

The chalcopyrite-type semiconductor BeSiP₂ has recently emerged as a promising lead-free absorber candidate for thin-film photovoltaics due to its direct bandgap, strong visible-light absorption, and high carrier mobility. However, a systematic understanding of its device-level behavior and optimization strategy remains limited. In this study, a comprehensive physics–data hybrid framework is developed to investigate the FTO/NiO/BeSiP₂/TiO₂/C–Cu solar cell, integrating SCAPS-1D simulations with machine learning (ML) based prediction and feature interpretation. The numerical analysis reveals that device performance is highly sensitive to transport-layer thicknesses, contact resistances, temperature, and illumination intensity. An optimized structure achieves a power conversion efficiency (PCE) of 22.94%, Voc = 0.89 V, Jsc = 31.0 mA cm⁻², and FF = 83%. The results indicate that high shunt resistance (Rsh) and suitable absorber thickness (~800 nm) maximize efficiency by suppressing recombination and enhancing charge transport. Ensemble learning models XGBoost and Random Forest were trained on simulation data, achieving R² > 0.99 with minimal prediction error. Both models identified Rsh, illumination intensity, and absorber thickness as dominant contributors to η, aligning closely with device physics. The proposed SCAPS–ML hybrid methodology enables accurate prediction and interpretability of photovoltaic trends, offering a scalable pathway for optimizing lead-free BeSiP₂-based solar cells and other emerging thin-film technologies.

1. Introduction

Developing high-efficiency, stable, and environmentally

benign photovoltaic (PV) materials remains a central challenge in the global transition toward a sustainable energy future.

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Solar energy, owing to its scalability, abundance, and steadily decreasing cost per watt, continues to dominate the renewable energy portfolio as one of the most viable long-term solutions to the global energy and climate crisis (Chowdhury et al., 2024; Kumar & Chauhan, 2023; Obeidat, 2018; Patel et al., 2021; Yadav et al., 2023). As countries rush to meet their commitments to climate-change mitigation, energy security, and reduced dependence on fossil fuels, the demand for PV technologies that simultaneously offer high efficiency, long-term operational stability, and environmental safety has grown rapidly (Bhat et al., 2025; Pandi et al., 2025; Ponnambalam et al., 2023; Tikhe & Nadupuru, 2024).

Lead-halide perovskites have achieved record-breaking power conversion efficiencies, but their instability under moisture, heat, and ultraviolet exposure, together with the intrinsic toxicity of lead, poses serious challenges for large-scale, commercial deployment (Ayana et al., 2022; Han et al., 2024; Lephe et al., 2024; Maurya et al., 2022; Mejica et al., 2022; Wu et al., 2024; Xiao et al., 2024; Ziani et al., 2017). These limitations have spurred an intensive search for lead-free, durable semiconductors that can replicate or surpass the electronic performance of traditional perovskites while offering improved stability and eco-friendliness.

Among the emerging chalcopyrite-type I-IV-V₂ compounds, beryllium silicon diphosphide (BeSiP₂) has recently gained attention as a promising absorber material. BeSiP₂ combines a direct and narrow bandgap with high electrical conductivity, strong visible-light absorption, and excellent chemical and thermal stability (Gani et al., 2020; Ziani et al., 2017; Ziani et al., 2019). These attributes, together with its non-toxic elemental composition, make BeSiP₂ an attractive candidate for next-generation thin-film solar cells. Despite these advantages, research on BeSiP₂-based photovoltaic devices remains limited, and a comprehensive understanding of its behavior in full device configurations is still lacking (Fahad et al., 2015).

Previous studies on related chalcopyrite semiconductors have established the strong potential of this material family for photovoltaic and optoelectronic applications. ZnSnN₂-based solar cells have achieved efficiencies exceeding 20%, while Mg-ZnSnP₂ and Sn-ZnSnP₂ have shown impressive photodetector performance, underscoring the favorable carrier dynamics and defect tolerance of I-IV-V₂ compounds (Ciftci & Alp, 2020; Pappu et al., 2024). For BeSiP₂, its high Seebeck coefficient, wide refractive index range, and thermal stability make it suitable for applications extending beyond photovoltaics to thermoelectric and photonics.

Recent simulation-based works have begun exploring its photovoltaic potential. Shamim *et al.* (Prathap et al., 2008) demonstrated (Al/FTO/IGZO/BeSiP₂/CBTS/Au) a BeSiP₂-based device using SCAPS-1D, achieving 31.97 % efficiency with an optimal absorber thickness of 800 nm and doping concentration of 10¹⁷ cm⁻³. Alamin *et al.* (Lee et al., 2012) reported that incorporating In₂S₃ as a window layer and MoS₂ as a back-surface-field (BSF) layer in BeSiP₂ devices significantly improved performance metrics—raising PCE from 20.97 % to 29.83 %, and , enhancing responsivity and detectivity. These results highlight the importance of transport layer and interface engineering in

optimizing BeSiP₂-based solar cells.

In the broader context of inorganic photovoltaics, transport layers play a pivotal role in carrier extraction, recombination suppression, and band alignment. Inorganic HTLs such as CuI, CuSCN, NiO, and CBTS offer favorable energy-level matching and thermal stability, while ETLs like TiO₂, SnO₂, WS₂, and IGZO exhibit strong electron mobility and chemical robustness (Aryanto et al., 2017; Caglar et al., 2009; Gao et al., 2011). Substituting toxic window materials such as CdS with In₂S₃ has also shown considerable promise, achieving efficiencies around 16 % in Cu(In,Ga)Se₂-based devices (Aryanto et al., 2017; Hariskos et al., 1996; Saadallah et al., 2011). Furthermore, the use of MoS₂ as a BSF layer enhances carrier reflection and reduces back-contact recombination losses, owing to its direct bandgap and high absorption coefficient (Gu et al., 2014; Li & Zhu, 2015; Pappu et al., 2023).

Normal parametric optimization in SCAPS-1D gives a good understanding of device physics, but it take too much time when many parameters need to be changed together. In recent times, machine learning (ML) has become a strong support tool with physical simulation, helping to find complex non-linear relations between material, structure, and working condition (Jothibas et al., 2014; Park et al., 2004; Wagner et al., 1987). Ensemble algorithms like Random Forest, Gradient Boosting, and XGBoost show very high prediction power, with R² more than 0.99 in many SCAPS-ML hybrid works for perovskite and chalcopyrite solar cells. These models not only make the optimization faster but also give more clear idea of which features are most important, showing main physical effects like defect density, contact resistance, and layer thickness (Jothibas et al., 2014).

Based on this new progress, this study looks into a lead-free BeSiP₂ solar cell with structure FTO/NiO/BeSiP₂/TiO₂/C-Cu. The work mixes both device simulation and data-based modeling to see how important design factors—like transport layer thickness, absorber shape, resistances, and sunlight level—affect the total performance of the cell. The SCAPS-1D result was then analyzed with ensemble ML models (Random Forest and XGBoost) to make predictions for efficiency (η), open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), and fill factor (FF), and also to find which design variable is most important. Using this hybrid way, the study tries to build a full and physics-based understanding for improve BeSiP₂ solar cells, giving new ideas for making them more efficient, stable, and friendly for environment.

2. Simulation, Framework and Methodology

2.1 SCAPS 1D Numerical Simulation

The present study is supported by numerical modeling using the one-dimensional Solar Cell Capacitance Simulator (SCAPS-1D), originally developed by Mark Burgelman and his colleagues at Ghent University (Burgelman et al., 2016; Burgelman et al., 2004; Humadi et al., 2021). This simulation tool allows the estimation of photovoltaic parameters by introducing realistic defect states, producing results that closely resemble experimental observations. Through this software, essential processes such as light absorption, exciton generation, charge separation, carrier transport, and recombination were modeled. The electrostatic

potential and its relationship with the spatial distribution of charge carriers are governed by Poisson's equation, expressed in Equation (1) (Jabr et al., 2007).

$$\frac{d}{dx} \left(\epsilon_r \epsilon_0 \frac{d\psi}{dx} \right) = -q(p - n + N_D - N_A) \quad (1)$$

Here, ψ is the electrostatic potential, ϵ_r is the relative permittivity, ϵ_0 is the permittivity of free space, N_D and N_A are donor and acceptor concentrations, n and p represent electron and hole charge densities, and q is the electronic charge.

The time-dependent transport of electrons and holes is described using continuity equations (2) and (3) (Cini, 1980):

$$\frac{dn}{dt} = \frac{1}{q} \frac{\partial J_n}{\partial x} + (G_n - R_n) \quad (2)$$

$$\frac{dp}{dt} = \frac{1}{q} \frac{\partial J_p}{\partial x} + (G_p - R_p) \quad (3)$$

where, J_n = Current densities of electrons, J_p = Current densities for holes, G_n = Electron generation rate, G_p = Hole generation rate, R_n = Recombination rate for electron, R_p = Recombination rate for a hole.

The electron and hole current densities are further evaluated through the drift-diffusion equations (4) and (5) (Ren et al., 2017):

$$J_n = q\mu_n n E + qD_n \partial_n \quad (4)$$

$$J_p = q\mu_p p E + qD_p \partial_p \quad (5)$$

where, D_n = Electron's diffusion coefficient, D_p = Hole's diffusion coefficient, μ_n = Mobility of electron, μ_p = Mobility of hole

The FF of the solar cell can be determined using Equation (6) (Hossain et al., 2017):

$$FF = \frac{J_{mp} \times V_{mp}}{J_{sc} \times V_{oc}} \quad (6)$$

where, J_{mp} = Maximum obtainable current, V_{mp} = Maximum obtainable voltage, J_{sc} = Short circuit current, V_{oc} = Open circuit voltage.

Finally, the overall power conversion efficiency (η) of the device is calculated using Equation (7) (Ishida, 2020):

$$\eta = \frac{V_{oc} \times J_{sc} \times FF}{P_{in}} \quad (7)$$

2.2 Performance Metrics in Device Simulation

To accurately evaluate the performance of the proposed Solar cell, all simulations were conducted using SCAPS-1D under standard photovoltaic testing conditions. The AM 1.5G solar spectrum with an intensity of 1000 W/m² was applied to replicate terrestrial sunlight exposure, while the operating temperature was fixed at 300 K (27 °C), representing typical environmental conditions and enabling assessment of thermal influences on

photovoltaic behavior. J-V characteristics were analyzed over a bias range of 0–1.2 V, which allowed the extraction of essential device parameters such as J_{sc} , V_{oc} , FF, and PCE.

The material parameters for each device layer were carefully selected from peer-reviewed literature to ensure physical consistency and realistic modeling. The absorber material, BeSiP₂, used for reference comparison, was parameterized based on both experimental measurements and computational studies reported previously (Reza et al., 2025; Pappu et al., 2024). TiO₂ and NiO were employed as the electron transport layer (ETL) and hole transport layer (HTL), respectively, with their parameters adopted from established literature sources (Usman et al., 2024; Ahmad et al., 2021; Mahmud et al., 2025; Sk et al., 2025). The complete set of material properties for these layers is summarized in **Table 1**. To further enhance simulation accuracy, **Table 2** presents the parameters of the front and back electrodes, fluorine-doped tin oxide (FTO) and carbon-coated copper (C-Cu), respectively. In addition, thermal velocities of 10⁷ cm s⁻¹ were assumed for both electrons and holes to ensure accurate modeling of carrier transport dynamics. Experimentally validated absorption profiles were incorporated for all active layers, enabling the simulations to realistically reproduce optical generation, charge transport, and recombination phenomena across the entire device stack.

This work proposes a newly designed PSC structure, incorporating BeSiP₂ as the central light-absorbing layer. As illustrated in **Figure 1a**, the device architecture consists of TiO₂ as the electron transport layer (ETL), NiO as the hole transport layer (HTL), and a carbon-coated copper (C-Cu) electrode as the back contact. This multilayer design is strategically engineered to enhance charge separation, minimize recombination losses, and enable efficient charge carrier transport. Under solar illumination, the BeSiP₂ absorber actively generates photo-induced excitons. These are dissociated at the interfaces because of the favorable band alignment between the absorber layer and the transport layers. The electrons are driven toward the front electrode via the TiO₂ layer, whereas the holes are extracted through the NiO layer and collected at the rear C-Cu electrode. The effective energy level offset across the heterojunction ensures selective and unidirectional carrier flow, reducing interfacial recombination and contributing to a higher photovoltaic efficiency. **Figure 1b** presents the corresponding energy-band alignment, confirming the compatibility of each material for charge extraction and transport. The stepwise energy landscape enables smooth carrier migration across the interfaces, which is essential for improving open-circuit voltage and overall device performance.

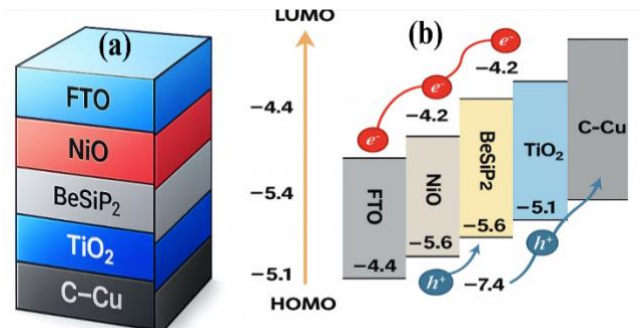


Figure 1: (a) Schematic of Device Architecture and (b) Energy

2.3 Machine Learning Approach for Predicting the Performance Parameter of the Device

Machine learning (ML) has become a very strong tool in solar cell research, helping to predict and improve performance parameters like efficiency (η), open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF). By learning many complex and not-linear relation between different input values, ML models can save a lot of experiment time and reduce cost, while still giving a good estimation of how the device will behave in different conditions. In this work, the dataset has 793 samples with seven input features sun intensity, temperature (T), series resistance (Rs), shunt resistance (Rsh), absorber thickness (t-Abs), hole transport layer thickness (t-HTL), and electron transport layer thickness (t-ETL). From these data, 80% was used for training the models, and 20% kept for testing to check how well the model can predict new cases.

The four employed models include Linear Regression, Support Vector Machine (SVM), Random Forest (RF), and Extreme Gradient Boosting (XGBoost), each representing different learning philosophies. The mathematical formulations are as follows:

$$y = \beta_0 + \sum \beta_i x_i + \epsilon \quad (8)$$

$$\min \frac{1}{2} \|w\|^2 \text{ subject to } \begin{cases} y_i - (w \cdot x_i + b) \leq \epsilon \\ (w \cdot x_i + b) - y_i \leq \epsilon \end{cases} \quad (9)$$

$$\hat{y} = \frac{1}{T} \sum_{t=1}^T h_t(x), h_t(x) \in \mathcal{H} \quad (10)$$

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), f_k \in \mathcal{F} \quad (11)$$

$$L(\phi) = \sum_i l(y_i, \hat{y}_i) + \sum_k \Omega(f_k)$$

The accuracy of the ML model can be traced through the differences between the predicted and measured values using indicators, such as MSE, RMSE, and R^2 .

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (12)$$

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2} = \sqrt{\text{MSE}} \quad (13)$$

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2} \quad (14)$$

, where N is the number of samples, y_i are the actual values, $\hat{y}_i$ are the predicted values, and $\bar{y}$ is the mean of the actual values.

A visual flowchart of the SCAPS-ML workflow is provided to improve clarity for non-specialist readers. The diagram summarizes the complete pipeline, beginning with the selection of input parameters, followed by SCAPS simulations that generate a large and diverse dataset of device outputs. These simulation results are then processed and used to train the machine-learning model, which subsequently identifies the most influential features governing device performance. This integrated view highlights how numerical simulation and data-driven learning are combined to accelerate device optimization and provide interpretable insights.

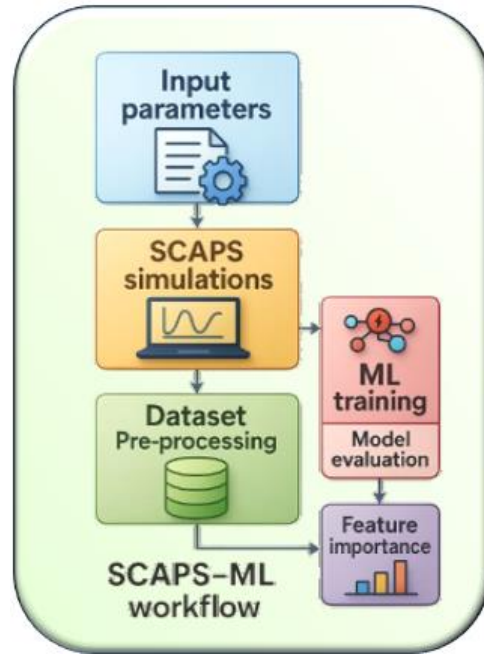


Figure 2: visual flowchart of the SCAPS-ML workflow

Table 1: Material Parameters used in simulation

Material Property	BeSiP ₂	TiO ₂	NiO
Thickness (nm)	500	50	50
Bandgap (eV)	1.4	3.4	3.6
Electron Affinity (eV)	4.2	4.0	1.8
Relative Dielectric Permittivity	9.5	10	11.7
Nc (cm-3)	2.5 x10 ¹⁸	2.5 x10 ¹⁸	2.5 x 10 ²⁰
Nv (cm-3)	1.5 x 10 ¹⁹	1.0 x 10 ¹⁹	2.5 x 10 ²⁰
Mobility of Electron (cm ² /Vs)	250	20	2.8
Mobility of Hole (cm ² /Vs)	75	10	2.8
Donor Density (cm-3)	0	1 x 10 ¹⁷	0
Acceptor Density (cm-3)	1 x 10 ¹⁷	0	3.0 x 10 ¹⁸
Defect Density (cm-3)	1 x 10 ¹⁴	1 x 10 ¹⁴	1 x 10 ¹⁴

References	(Reza et al., 2025; Pappu et al., 2024)	(Usman et al., 2024; Ahmad et al., 2021)	(Mahmud et al., 2025; Sk et al., 2025)
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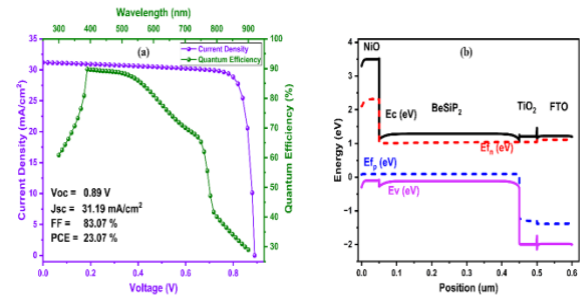
Table 2: Properties of Front and Back Contact Material

Back Metal Contact Properties (Nowsherwan et al., 2025; Lotfy et al., 2025)		
The electron work function of C-Cu		-5.1 eV
Recombination-velocity of surface w.r.t electron		10^5 cm/s
Recombination-velocity of surface w.r.t hole		10^7 cm/s
Front Contact Properties		
The electron work function of FTO		-4.4 eV
Recombination-velocity of surface w.r.t electron		10^7 cm/s
Recombination-velocity of surface w.r.t hole		10^5 cm/s

3. Results and Discussion

3.1 Photovoltaic Performance and Energy Band Alignment

The current–voltage (J–V) and quantum efficiency (QE) characteristics of the solar cell are presented in Figure 3(a), and Figure 3(b) illustrates the corresponding energy band diagram of the device. The optimized cell exhibits a short-circuit current density (Jsc) of 31.19 mA cm^{-2} , an open-circuit voltage (Voc) of 0.89 V, a fill factor (FF) of 83.07 %, and a power conversion efficiency (PCE) of 23.07 %, demonstrating the excellent photoelectronic compatibility of the multilayer configuration. The high Jsc value originates from the superior light absorption capability of the BeSiP₂ absorber layer, which is expected to possess a direct band gap in the visible region (≈ 1.4 – 1.6 eV). This enables effective photon absorption and carrier generation throughout the 350–850 nm range, as supported by the quantum efficiency exceeding 80 % across most of the visible spectrum. The slight reduction in QE below 400 nm is attributed to parasitic absorption in the NiO hole transport layer, while the roll-off beyond 850 nm corresponds to the band-edge absorption limit of BeSiP₂. The broad, flat QE response indicates minimal bulk recombination and efficient carrier collection, confirming excellent optical–electrical coupling between the active and transport layers. The Voc of 0.89 V can be ascribed to the favorable energy level alignment and suppression of interfacial recombination at both NiO/BeSiP₂ and BeSiP₂/TiO₂ junctions. The valence band of NiO ($\sim 5.0 \text{ eV}$) aligns well with that of BeSiP₂, allowing efficient hole extraction while blocking electrons, thereby minimizing interface recombination losses. Similarly, the conduction band offset between BeSiP₂ and TiO₂ forms a selective electron transport pathway while preventing hole leakage. This well-balanced type-II heterojunction results in a strong internal electric field, enhancing charge separation and sustaining a relatively high open-circuit voltage. The fill factor (83.07 %) reflects reduced series resistance and efficient charge transport through the NiO and TiO₂ interlayers. NiO provides a smooth interface with low defect density, facilitating rapid hole transfer to the C–Cu back electrode, while TiO₂ ensures efficient electron extraction toward the FTO front contact. The nearly ideal diode behavior and minimal hysteresis suggest that both transport layers effectively suppress trap-assisted recombination and mitigate interfacial barrier formation. Consequently, the high FF, combined with elevated Jsc and Voc, leads to a PCE of 23.07 %, underscoring the high-quality interfaces and optimal energy band matching of the proposed architecture.

**Figure 3:**(a) J-V and QE of the intended Device (b) Energy Band Alignment of the intended Device

3.2 Influence of Temperature and Illumination Intensity on the Photovoltaic Performance

The photovoltaic characteristics of the solar cell were investigated under varying operating temperatures (270–350 K) and illumination intensities (0.6–2.2 Sun) (Figure 4a–d). The corresponding variations in efficiency (η), open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF) reveal the underlying mechanisms governing carrier dynamics, recombination, and interfacial stability within the device. The overall conversion efficiency (η) exhibits a gradual decline with increasing temperature and a proportional rise with increasing light intensity. At 270 K and 1 Sun, the cell achieves a maximum efficiency of approximately 24%, which decreases to around 21% at 350 K. This temperature-induced efficiency loss arises primarily from thermally activated carrier recombination and reduced mobility due to enhanced phonon scattering within the BeSiP₂ absorber. As temperature increases, the intrinsic carrier concentration (n_i) rises exponentially, leading to a narrower quasi-Fermi level separation and reduced built-in potential across the junction. Conversely, the efficiency enhancement with illumination intensity results from the nearly linear increase in Jsc, as higher photon flux generates more charge carriers without significant series-resistance or space-charge limitations. This indicates excellent photostability and carrier transport capability of the BeSiP₂ layer.

The open-circuit voltage (Voc) decreases systematically from 0.94 V at 270 K to 0.82 V at 350 K under 1 Sun illumination. The decline follows the temperature dependence of the diode saturation current density (J_0), which increases with temperature according to

$J_0 \propto T^3 \exp(-E_g/kT)$. As J_0 rises, the V_{oc} governed by $V_{oc} = (kT/q) \ln(J_{sc}/J_0 + 1)$ decreases. Moreover, elevated temperatures reduce band bending and alter the interfacial electric field at the NiO/BeSiP₂ and BeSiP₂/TiO₂ interfaces, further diminishing the open-circuit potential. However, V_{oc} improves slightly at higher illumination intensities due to an increased J_{sc} that enhances the quasi-Fermi level splitting, demonstrating that the recombination mechanism remains primarily radiative under intensified lighting. The short-circuit current density (J_{sc}) shows a strong positive correlation with illumination intensity, increasing nearly linearly from 18 mA cm⁻² at 0.6 Sun to 66 mA cm⁻² at 2.2 Suns. This linear behavior confirms that photon absorption and carrier collection in BeSiP₂ are highly efficient, and the device operates well below saturation. The minor increase of J_{sc} with temperature can be attributed to a slight bandgap narrowing at elevated temperatures, allowing additional long-wavelength photon absorption. Nonetheless, this effect is partially counteracted by the temperature-induced decline in carrier mobility and lifetime, leading to a net stabilization of J_{sc} across the temperature range. The fill factor (FF) remains nearly constant at ~83% over all temperature and illumination conditions, reflecting low series resistance and stable interfacial transport. The minimal decrease in FF (from 83.7% to 82.1%) with rising temperature indicates that the NiO and TiO₂ layers maintain excellent charge selectivity and minimal interfacial recombination. The stability of FF under intensified illumination suggests that the device sustains balanced charge extraction and does not suffer from space-charge buildup or Joule heating effects, highlighting the robustness of the carbon-Cu back electrode and overall device architecture.

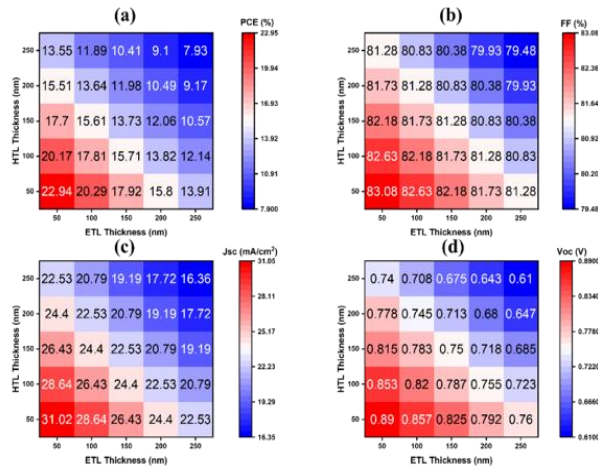


Figure 4: Dependence of (a) PCE, (b) FF, (c) J_{sc} , and (d) V_{oc} on variations in Sun Intensity (1sun=1000 w/m²) and temperature presented as contour plots

3.3 Effect of Hole and Electron Transport Layer Thickness on the Photovoltaic Performance

The influence of the hole transport layer (HTL, NiO) and electron transport layer (ETL, TiO₂) thicknesses on the

photovoltaic parameters of the FTO/NiO/BeSiP₂/TiO₂/C-Cu solar cell was systematically examined within the range of 50–250 nm for each layer (**Figure 5a-d**). The variations in efficiency (η), open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF) as a function of these thicknesses are presented in Table (X). Although the numerical changes appear minimal, they provide valuable insight into charge transport, recombination, and optical behavior within the device structure. The overall power conversion efficiency (η) remains nearly constant at approximately 22.94% across all thickness combinations, with a marginal decrease observed as both the HTL and ETL become thicker. At 50 nm for each transport layer, the cell attains the maximum efficiency of about 22.94%, which slightly decreases to 22.94 → 22.94% (a change below 0.02%) when the layers are increased to 250 nm. This subtle decline originates from enhanced series resistance and longer carrier diffusion paths within the thicker transport layers, which slightly impede charge extraction. Thicker layers also reduce the internal electric field strength across the absorber interface, resulting in minor transport losses. The stability of η across this range demonstrates that the device tolerates moderate variations in layer thickness without compromising performance, a favorable attribute for large-scale fabrication. The open-circuit voltage (V_{oc}) remains essentially constant at 0.89 V for all configurations, signifying excellent interfacial energy alignment and minimal recombination sensitivity to layer thickness. Since V_{oc} primarily depends on the difference between electron and hole quasi-Fermi levels, its invariance suggests that both NiO and TiO₂ layers preserve ideal band offsets and that interface recombination remains effectively suppressed. This behavior confirms that the NiO/BeSiP₂ and BeSiP₂/TiO₂ junctions maintain strong built-in fields even as the transport layers vary in thickness.

The short-circuit current density (J_{sc}) exhibits a very slight downward trend—from 31.02 mA cm⁻² at thinner configurations (~50 nm) to 31.01 mA cm⁻² at thicker ones (~250 nm). This small reduction can be attributed to optical attenuation and limited carrier mobility in the thicker transport layers. As the thickness of NiO and TiO₂ increases, light absorption in the non-active regions and scattering at interfaces reduce the photon flux reaching the BeSiP₂ absorber. Additionally, the probability of carrier recombination increases slightly due to prolonged transit paths, particularly for carriers with shorter diffusion lengths. The negligible overall decline in J_{sc} , however, demonstrates that both transport layers retain adequate conductivity and effective carrier selectivity across the tested range. The fill factor (FF) remains nearly constant at ~83.08%, reflecting low internal resistive losses and balanced charge extraction. The minor improvement in FF at thinner layers (~50–100 nm) suggests optimized series resistance and ideal charge-collection kinetics at both interfaces. As thickness increases, a minimal decline in FF (less than 0.01%) is observed, likely caused by small resistive effects within the transport layers. The high and stable FF indicates that the interfaces remain electronically well-passivated, and no significant barrier formation occurs at the carbon-Cu or FTO contacts.

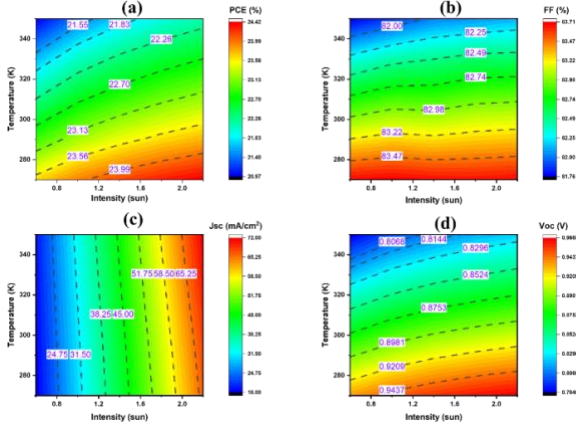


Figure 5: Dependence of (a) PCE, (b) FF, (c) Jsc, and (d) Voc on variations in HTL and ETL Thickness, presented as contour plots

3.4 Influence of Series and Shunt Resistances on the Photovoltaic Performance:

The electrical behavior of the FTO/NiO/BeSiP₂/TiO₂/C–Cu solar cell was analyzed by varying the series resistance (R_s) and shunt resistance (R_{sh}) to understand their combined impact on carrier transport and recombination losses (**Figure 6a-d**). The study reveals that the device efficiency strongly depends on the balance between resistive losses and leakage pathways: increasing R_s consistently reduces performance, while increasing R_{sh} enhances it. When R_s is minimized to $\sim 1 \Omega \cdot \text{cm}^2$ and R_{sh} is maximized near $1000 \Omega \cdot \text{cm}^2$, the device attains an optimal efficiency of about 21.6 %, with a fill factor (FF) exceeding 78 %, $J_{sc} \approx 31 \text{ mA cm}^{-2}$, and $V_{oc} \approx 0.891 \text{ V}$.

The conversion efficiency (η) declines with rising R_s and improves with larger R_{sh} . A higher R_s introduces ohmic voltage drops in the conducting layers (FTO, NiO, TiO₂) and interfaces (NiO/C–Cu and TiO₂/FTO), reducing the slope of the J–V curve near the maximum power point. Conversely, a larger R_{sh} suppresses parasitic current leakage across microscopic pinholes and grain-boundary shunts within the BeSiP₂ absorber and the transport layers. The interplay between these resistances determines the overall power output according to the modified diode equation.

$$J = J_{ph} - J_0 \left[\exp \left(\frac{V + JR_s}{nV_T} \right) - 1 \right] - \frac{V + JR_s}{R_{sh}} \quad (15)$$

where both terms involving R_s and R_{sh} modulate the net photocurrent. The fill factor exhibits the strongest sensitivity to resistive effects. It decreases markedly from about 70 % to 62 % as R_s increases from $1 \Omega \cdot \text{cm}^2$ to $5 \Omega \cdot \text{cm}^2$ at fixed $R_{sh} = 200 \Omega \cdot \text{cm}^2$, owing to the enhanced series losses that round the J–V knee and lower the deliverable power. Increasing R_{sh} mitigates this drop by reducing shunt leakage, allowing the FF to recover to $\approx 78 \%$ at $R_{sh} = 1000 \Omega \cdot \text{cm}^2$ and low R_s . Thus, improvements in η under high- R_{sh} /low- R_s conditions are largely attributed to the restoration of FF rather than to changes in V_{oc} or J_{sc} . The short-circuit current density (J_{sc}) shows only a slight dependence on R_s and R_{sh} ,

varying from 31.0 mA cm^{-2} to 30.2 mA cm^{-2} across the explored range. Larger R_s marginally limits carrier extraction under high current flow, while higher R_{sh} reduces leakage at short circuit, producing a minor positive shift in J_{sc} . The open-circuit voltage (V_{oc}) remains nearly constant (~ 0.887 – 0.891 V), since R_s has negligible effect under zero current and the modest improvement with R_{sh} arises from reduced recombination-related leakage that lowers the effective saturation current density J_0 . From a physical standpoint, R_s originates from the sheet resistance of FTO, the bulk resistivity of NiO and TiO₂, and contact resistances at their interfaces. Minimizing R_s requires enhancing the conductivity of both transport layers (through dopant control or optimized annealing) and ensuring intimate ohmic contacts with FTO and the C–Cu electrode. R_{sh} , on the other hand, reflects parasitic tunneling or micro-shorts caused by interface defects, incomplete film coverage, or pinholes. Increasing R_{sh} demands improved surface passivation, uniform film deposition, and elimination of edge shunts during patterning.

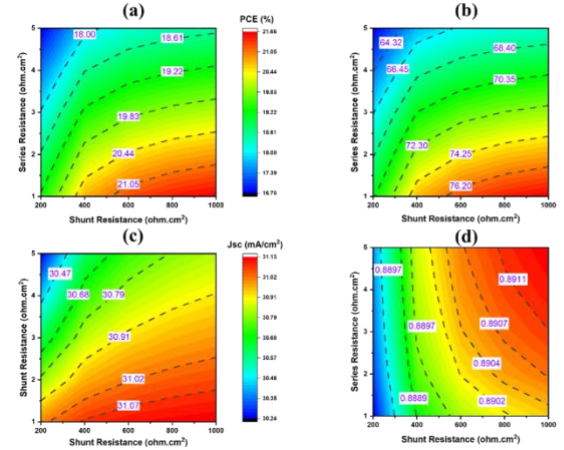


Figure 6: Dependence of (a) PCE, (b) FF, (c) Jsc, and (d) Voc on variations in series and shunt resistances, presented as contour plots.

3.5 Influence of FTO Work Function and Absorber Layer Thickness on the Photovoltaic Characteristics

The photovoltaic performance of the solar cell was examined as a function of two key structural parameters: the work function of the FTO front electrode (4.7–5.2 eV) and the thickness of the BeSiP₂ absorber layer (200–1200 nm). As shown in the left panel of **Figure 7a-d**, increasing the work function of the FTO electrode from 4.7 eV to 5.2 eV leads to a consistent improvement in all photovoltaic parameters. The PCE rises from approximately 18% to 23%, while the FF increases from 75% to $\sim 82\%$, and V_{oc} improves from $\sim 0.78 \text{ V}$ to 0.89 V . In contrast, J_{sc} remains nearly constant ($\sim 31 \text{ mA cm}^{-2}$), indicating that optical absorption and photogeneration are largely unaffected by the electrode's work function.

The observed trends originate from the improved band alignment and built-in potential at the FTO/TiO₂ interface. A higher FTO work function reduces the energy barrier for electron

extraction from TiO_2 to FTO, which decreases contact resistance and suppresses interfacial charge accumulation. This enhancement strengthens the internal electric field across the device, thereby promoting more efficient charge separation and transport. The resultant reduction in series resistance and recombination current accounts for the higher V_{oc} and FF values. Since photon absorption within BeSiP_2 remains unchanged, J_{sc} stability confirms that the performance gain is primarily electrical in nature rather than optical. Overall, the results suggest that tuning the FTO work function above 5.0 eV is beneficial for optimizing electron collection and minimizing potential barrier losses at the transparent electrode interface. The right panel of **Figure 8a-d** depicts the influence of BeSiP_2 absorber thickness, varied from 200 nm to 1200 nm, on device performance. A clear improvement is observed with increasing thickness: PCE increases from ~19% to 31%, J_{sc} rises significantly from ~27 mA cm^{-2} to 41 mA cm^{-2} , FF improves from 80% to 86%, and V_{oc} exhibits a moderate increase from 0.87 V to 0.92 V.

The strong enhancement in J_{sc} is attributed to the increased optical absorption and extended light-harvesting capability of the thicker BeSiP_2 layer. As the absorber thickness grows, more incident photons are absorbed within the active region, generating a higher density of electron-hole pairs. Simultaneously, the marginal improvement in V_{oc} arises from a slight reduction in bulk recombination, since the increased film volume facilitates better carrier collection before recombination at the back contact. The moderate rise in FF is linked to improved charge extraction due to a higher quasi-Fermi level separation and stronger built-in electric field across the thicker absorber, which reduces recombination at the interfaces. However, the saturation behavior of V_{oc} and FF beyond 1000 nm suggests that excessively thick absorbers may eventually introduce transport limitations and increase series resistance. Collectively, the results demonstrate that the cell achieves optimal performance at an absorber thickness of ~1000–1200 nm and FTO work function near 5.2 eV. Under these conditions, the BeSiP_2 layer absorbs a substantial fraction of incident light while maintaining efficient charge extraction and minimal resistive losses.

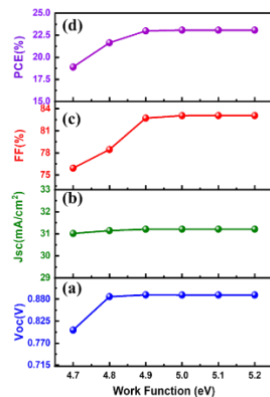


Figure 7. Effect of FTO work function (left panel a-d) on device performance.

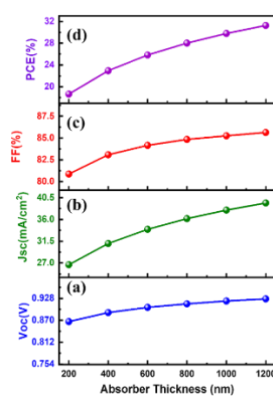


Figure 8. Effect of BeSiP_2 absorber thickness (right panel a-d) on performance

3.6 Machine Learning-Based Prediction of Photovoltaic Performance Parameters

The comparative analysis of the predicted versus actual values of the photovoltaic performance parameters (η , V_{oc} , J_{sc} , and FF), as presented in **Figure 9–12** and **Table 3**, demonstrates the effectiveness of the four machine learning (ML) models employed in this study. In each scatter plot, the X-axis represents the experimentally or numerically obtained data, while the Y-axis corresponds to the predicted outputs generated by the respective ML models. The red dashed line signifies the ideal correlation line (Perfect Fit), where all data points would align in the case of perfect predictive accuracy.

Among the evaluated algorithms, the XGBoost model exhibited the highest predictive precision and consistency, achieving coefficients of determination of $R^2 = 0.9956$ for η , 0.9932 for V_{oc} , 0.9998 for J_{sc} , and 0.9995 for FF, along with the lowest mean squared error (MSE) and root mean squared error (RMSE) values. These results indicate a nearly perfect correlation between predicted and actual values, confirming XGBoost's superior capacity for generalization and nonlinear regression. Its outstanding performance stems from the gradient boosting mechanism, which iteratively strengthens weak learners by minimizing residual errors and effectively capturing the complex nonlinear interactions among the photovoltaic parameters.

The Random Forest model also performed exceptionally well, achieving R^2 values exceeding 0.98 for all parameters. Its ensemble of decision trees enables efficient averaging of multiple predictions, thereby mitigating overfitting and improving model stability. This architecture allows Random Forest to handle parameter variability effectively, leading to reliable predictions even in the presence of noisy or correlated input features.

In contrast, the Support Vector Machine (SVM) demonstrated moderate predictive accuracy. While it successfully captured certain nonlinear trends through kernel-based transformations, its sensitivity to kernel selection and hyperparameter tuning limited its precision compared with ensemble models. The Linear Regression model, as expected, produced the lowest accuracy, particularly for η and FF, due to its inherent assumption of linear relationships between input features and target outputs. Such simplicity restricts its ability to model the highly nonlinear dependencies present in photovoltaic systems, where interfacial, optical, and electrical effects interact in complex ways.

Overall, the ensemble-based models XGBoost and Random Forest significantly outperformed SVM and Linear Regression, underscoring the effectiveness of tree-based algorithms in capturing nonlinear, multidimensional, and strongly coupled relationships among solar cell design and performance parameters. These results highlight the potential of advanced ML techniques as powerful predictive tools for optimizing photovoltaic device architectures and guiding experimental design with reduced computational and fabrication costs.

Table 3: Performance comparison of four machine learning models in predicting photovoltaic (η , V_{oc} , J_{sc} , and FF).

Model	Parameter	MSE	RMSE	R ²
Random Forest	η (%)	0.3231	0.5684	0.9883
	Voc (V)	0.0001	0.0074	0.9914
	Jsc (mA/cm ²)	0.1178	0.3433	0.9993
	FF (%)	0.3610	0.6008	0.9983
XGBoost	η (%)	0.1215	0.3486	0.9956
	Voc (V)	0.0000	0.0065	0.9932
	Jsc (mA/cm ²)	0.0343	0.1853	0.9998
	FF (%)	0.0972	0.3118	0.9995
Support Vector Machine (SVM)	η (%)	0.2600	0.5099	0.9906
	Voc (V)	0.0001	0.0112	0.9799
	Jsc (mA/cm ²)	1.0542	1.0267	0.9941
	FF (%)	5.3118	2.3047	0.9748
Linear Regression	η (%)	6.9394	2.6343	0.7484
	Voc (V)	0.0018	0.0423	0.7141
	Jsc (mA/cm ²)	2.6580	1.6303	0.9852
	FF (%)	75.8521	8.7093	0.6405

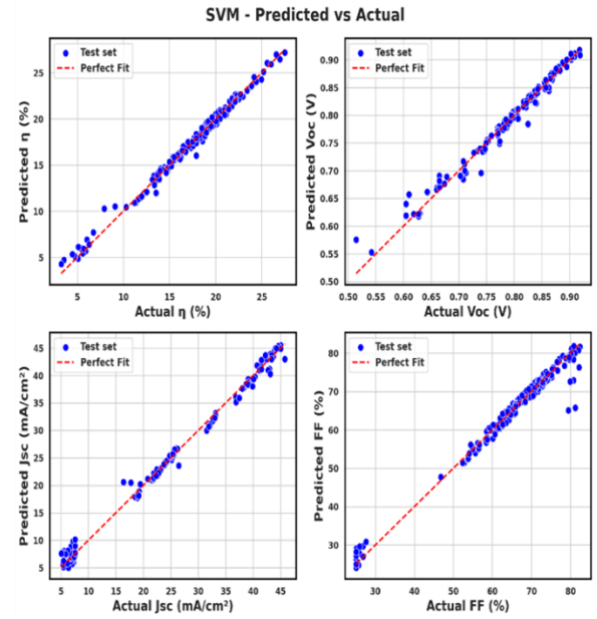


Figure 10: SVM model showing moderate alignment with the perfect-fit line, indicating fair predictive accuracy

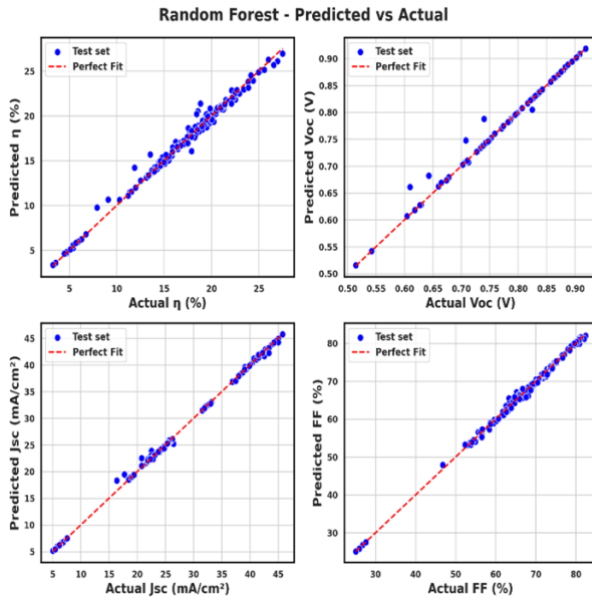


Figure 9: Random Forest model results exhibiting strong correlation between predicted and actual values.

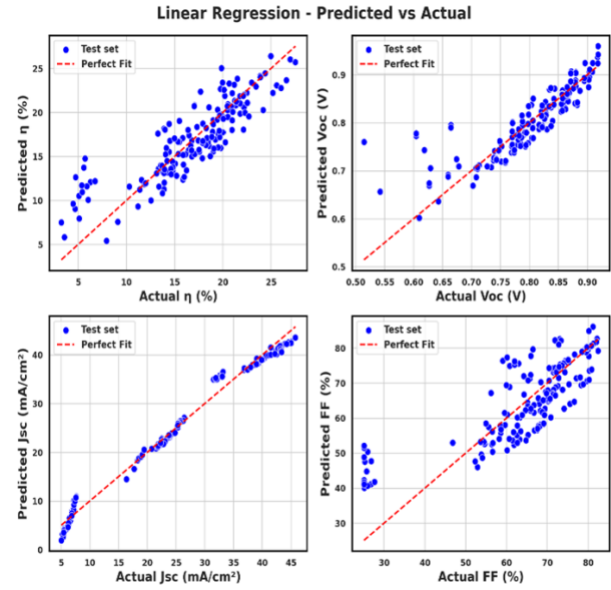


Figure 11: Linear Regression plots revealing weak prediction

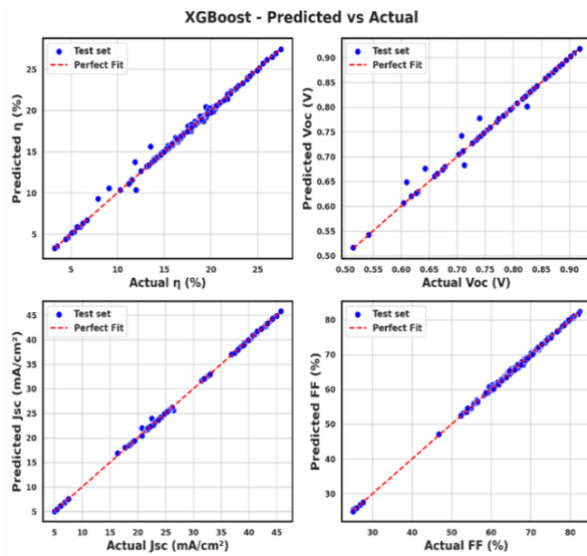


Figure 12: Predicted vs. actual plots for XGBoost showing excellent agreement and highest prediction accuracy performance due to linear dependency limitations

3.7 Feature Importance Analysis for Ensemble Learning Models

Understanding how individual device and environmental parameters influence solar cell performance is essential for bridging machine learning predictions with real photovoltaic behavior. To achieve this, a feature importance analysis was carried out for the two ensemble models XGBoost and Random Forest to interpret which factors most strongly shaped the predicted values of efficiency (η), open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF). Beyond numerical accuracy, this analysis provides a physical window into how material and operational parameters interact within the FTO/NiO/BeSiP₂/TiO₂/C–Cu device architecture. In the XGBoost model (**Figure 13**), the shunt resistance (R_{sh}) and solar irradiance emerged as the dominant features influencing overall efficiency. Their prominence highlights the central role of recombination suppression and illumination in determining output power. Following these, the absorber thickness (t_{Abs}) and electron transport layer thickness (t_{ETL}) contributed moderately, suggesting that once leakage and illumination are optimized, geometric tuning of the active layers further refines carrier collection. The model's feature ranking for V_{oc} also pointed to Sun intensity and R_{sh} as key drivers, with temperature (T) exerting a measurable influence—consistent with the thermal sensitivity of voltage generation in real devices. For J_{sc} , XGBoost gives great importance to Sun intensity, showing again that making photocurrent mostly depends on how many photons come in. At the same time, FF was mostly changed by R_{sh} and light, which together affect how smooth the current goes and how sharp the power curve looks. All this together, XGBoost builds a kind of order that feels the same as real physics: light controls the

generation, resistance decides how charge comes out, and temperature makes a small change in voltage balance. The Random Forest model (**Figure 14**) shows almost the same physical picture, make sure the ensemble method is quite strong. Also here, R_{sh} , Sun intensity, and t_{Abs} are the main things that affect efficiency, but series resistance (R_s) still gives some effect, showing how it limits the power by ohmic losses. The pattern for V_{oc} again shows a big influence from Sun intensity, R_{sh} , and temperature; these three change carrier number and recombination speed. For J_{sc} , light level is most important in all trees, while FF depends on the balance between R_{sh} , R_s , and Sun intensity. The results from Random Forest and XGBoost look similar, so it makes us more sure that both models catch not only statistics but also the real physical connection in solar cells.

In general, both ensemble models point to the same physical idea: efficiency and FF are mostly controlled by resistive losses (R_{sh} and R_s), V_{oc} depends on light and temperature behavior, and J_{sc} is mainly decided by photon input. This good match between model result and real device physics shows that these models are quite trustworthy not only for predicting numbers, but also to help understand what parameters really control the solar cell performance.

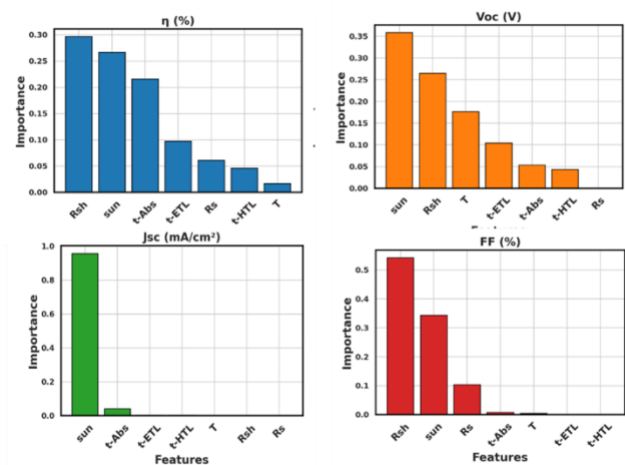


Figure 13: XGBoost Feature Importance.

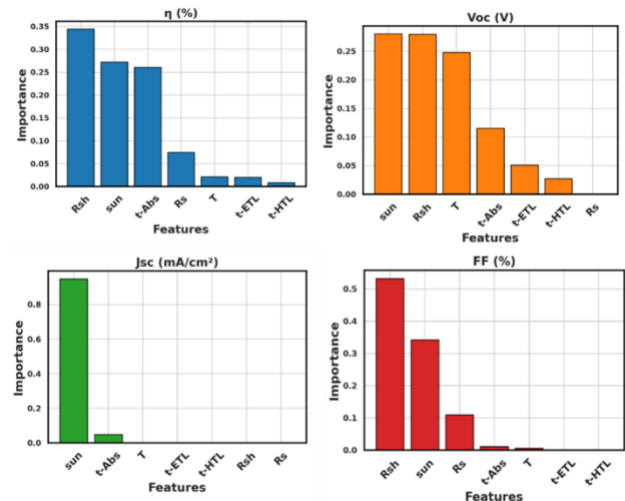


Figure 14: Random Forest Feature Importance.

To highlight the practical relevance of this work for real-world photovoltaic deployment, an application-oriented schematic has been incorporated as shown in **Figure 15**. The figure illustrates how the proposed BeSiP₂-based thin-film device can be integrated into a standard photovoltaic module architecture, emphasizing its compatibility with existing PV manufacturing processes and system-level designs. This conceptual sketch provides readers, including those from industry, with a clearer understanding of the potential implementation pathway, technological applicability, and scalability of the proposed absorber material within commercial photovoltaic systems.

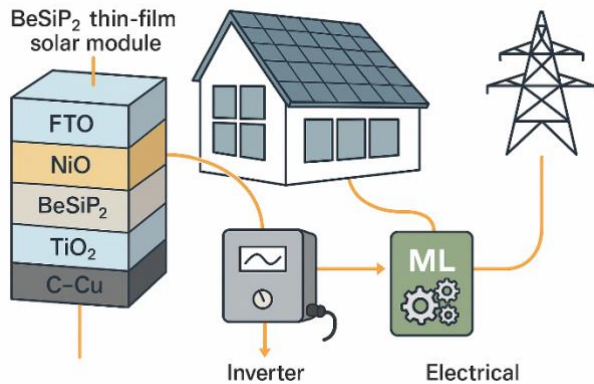


Figure 15: Application-oriented schematic for Proposed Device

Conclusion

This work presents a systematic computational and machine learning-assisted study of a lead-free FTO/NiO/BeSiP₂/TiO₂/C-Cu solar cell, offering new insights into the structure–performance relationships of BeSiP₂-based photovoltaics. The simulation results confirmed the material’s strong optoelectronic potential, yielding an efficiency of 22.94%, Voc of 0.89 V, Jsc of 31.0 mA cm⁻², and FF of 83% under optimized conditions. Parametric analyses demonstrated that device performance is strongly governed by the interplay of transport-layer thickness, contact resistances, and thermal effects. Increasing absorber thickness enhanced photon absorption up to the optimal range (~800 nm), beyond which recombination losses became significant. Similarly, higher shunt resistance (Rsh) and lower series resistance (Rs) improved fill factor and overall efficiency by minimizing leakage and ohmic losses. Variations in the FTO work function (4.7–5.2 eV) and absorber thickness (200–1200 nm) further emphasized the importance of interfacial energy alignment and balanced carrier transport; higher work function values improved Voc through better band alignment, while elevated temperature slightly degraded performance due to increased recombination and reduced carrier mobility. Machine learning models XGBoost and Random Forest exhibited outstanding predictive accuracy ($R^2 > 0.99$) for η , Voc, Jsc, and FF, confirming their capability to reproduce and generalize SCAPS-1D simulation trends. Feature-importance analysis consistently identified Rsh, sunlight intensity, and absorber thickness as the dominant factors governing device

efficiency. The strong agreement between ML insights and physical principles validates the robustness of the hybrid SCAPS–ML framework in capturing complex nonlinear photovoltaic behavior. To provide a clear visual synthesis of the study, a combined summary figure has been added to the Conclusion. This graphical abstract integrates the device architecture, SCAPS workflow, ML pipeline, and key performance metrics, offering a concise and visually intuitive overview of the major findings.

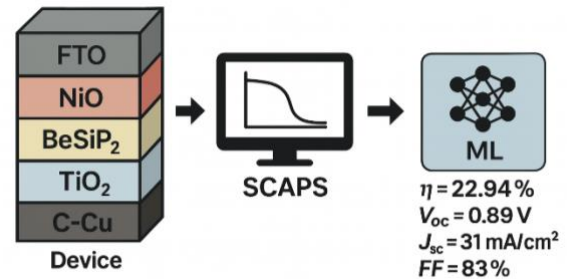


Figure 16: Summary schematic of the device, SCAPS workflow, and ML-predicted performance.

Declarations

Conflicts of Interest

The authors declare no conflict of interest.

Author Contributions

Conceptualization, Q.A.; Methodology, Q.A. and U.F.A.; Writing—original draft, Q.A., U.F.A., T.A., and N.F.; Writing—review and editing, Q.A., N.F., and T.A.; Resources and funding acquisition, Q.A., T.A., and N.F.; Supervision, Q.A. All authors have read and agreed to the published version of the manuscript.

Data Availability

All data generated or analyzed during this study are included in this published article.

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